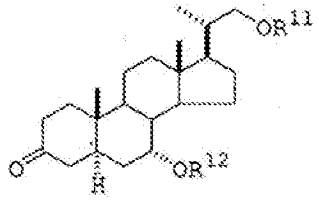
AMENDMENTS TO THE CLAIMS

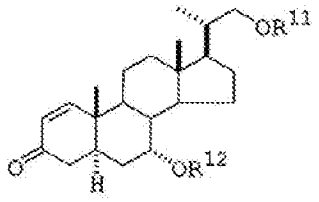
This listing of claims replaces all prior versions, and listings, of claims in the application.

1. (Original) A method for producing a mixture of a 5α-pregnane derivative represented by the formula (II):



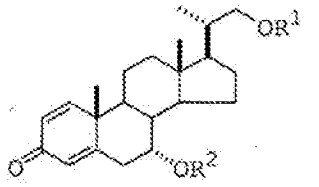
(II)

wherein R^{11} and R^{12} are each independently a hydrogen atom or a hydroxyl-protecting group, and a 5α-pregnane derivative represented by the formula (III):



(III)

wherein R^{11} and R^{12} are as defined above, which comprises reacting a pregnane derivative represented by the formula (I):



(I)

wherein R^1 is a hydroxyl-protecting group and R^2 is a hydrogen atom or a hydroxyl-protecting group, with a metal selected from alkali metals and alkaline earth metals in the presence of a proton donor and an amine and/or ammonia.

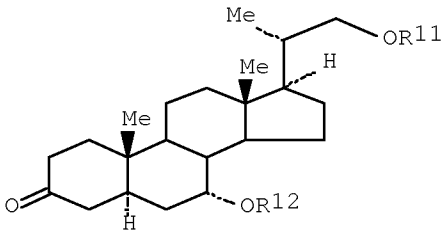
2. (Original) The method of claim 1, wherein R^2 and R^{12} are hydrogen atoms.

AUTHOR SEARCH

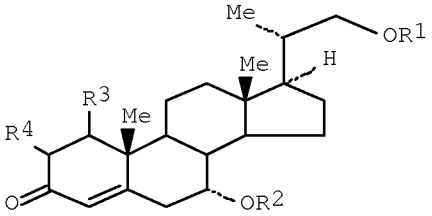
L18 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1106865 HCAPLUS Full-text
DOCUMENT NUMBER: 143:387237
TITLE: Process for the preparation of 5α-pregnane derivative via reduction of carbon-carbon double bond in pregn-4-en-3-one compound
INVENTOR(S): Sugioka, Takashi; Ohzono, Shigeo; Koyakumaru, Kenichi; Nakagawa, Naoshi
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095434	A1	20051013	WO 2005-JP6828	20050331
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1743902	A1	20070117	EP 2005-728917	20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1934124	A	20070321	CN 2005-80009530	20050331
US 20070149494	A1	20070628	US 2006-594164	20060926
IN 2006CN03994	A	20070706	IN 2006-CN3994	20061031
PRIORITY APPLN. INFO.:			JP 2004-108419 A	20040331
			WO 2005-JP6828 W	20050331

OTHER SOURCE(S): MARPAT 143:387237
ED Entered STN: 14 Oct 2005
GI



I



II

AB A process for the preparation of compound I [R11, R12 = H, protecting group of hydroxy], characterized by reduction a pregnane derivative II [R1 = protecting group of hydroxy; R2 = H, protecting group of hydroxy; R3 and R4 represent hydrogen atoms or combine together to form a bond.] with alkali metals or alkaline earth metals in the presence of a proton donor, amine and/or ammonia, was disclosed. For example, to a solution of (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methylpregn-4-en-3- one (5.00 g) and tert-butanol (1.78 g) in THF (100 mL) was added liquid ammonia (100 mL) at -50 °C. Then, Li metal (0.17 g) was added, while maintaining the reaction temperature between -50 and -40 °C, the reaction was stirred -40 °C for 3 h. The resulting reaction was treated with ammonium sulfate (1.59 g) followed by removal of ammonia, aqueous work-up and silica-gel purification to give (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methyl-5α- pregn-3-one in 96% yield. Of note compds. I are useful synthetic intermediates for the preparation of squalamine.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103797 HCAPLUS Full-text
DOCUMENT NUMBER: 143:387233
TITLE: Method for producing 5α-pregnane derivative
INVENTOR(S): Koyakumaru, Kenichi; Sugioka, Takashi; Ohzono, Shigeo; Nakagawa, Naoshi
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

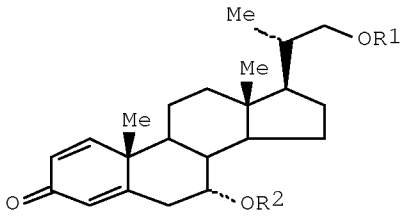
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095431	A1	20051013	WO 2005-JP6818	20050331

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CN 1938330	A	20070328	CN 2005-80010110		20050331
EP 1767540	A1	20070328	EP 2005-728889		20050331
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR					
US 20070197490	A1	20070823	US 2006-594163		20060926
IN 2006CN03996	A	20070706	IN 2006-CN3996		20061031
PRIORITY APPLN. INFO.:			JP 2004-108434	A	20040331
			WO 2005-JP6818	W	20050331

OTHER SOURCE(S): MARPAT 143:387233
ED Entered STN: 14 Oct 2005
GI



I

AB 5α-Pregna-3-one derivs. and 5α-pregna-1-en-3-one derivs. are prepared by reacting a pregnane derivative represented by the general formula I [R1 = OH-protecting group; R2 = H, OH-protecting group] with a metal selected from alkali metals and alkaline earth metals in the presence of a proton donor, an amine and/or ammonia. The title compds. are intermediates for squalamine. Thus, (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methyl-5α- pregna-3-one and (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20- methyl-5α-pregna-1-en-3-one were prepared by the title method.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

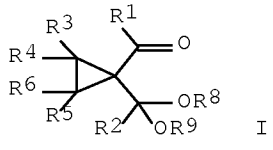
L18 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103727 HCAPLUS Full-text
DOCUMENT NUMBER: 143:386684
TITLE: Process for the preparation of cyclopropane monoacetal derivative and intermediate therefor
INVENTOR(S): Koyakumaru, Kenichi; Ueyama, Shingo; Ujita, Katsuji; Hayashibara, Tatsuhiko; Nakagawa, Naoshi; Akiba, Toshifumi; Saito, Tatsuru
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan; Daiichi Pharmaceutical Co., Ltd.
SOURCE: PCT Int. Appl., 24 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

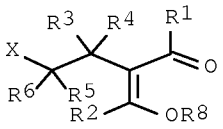
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095318	A1	20051013	WO 2005-JP6407	20050325
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1731495	A1	20061213	EP 2005-727496	20050325
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
US 20070191643	A1	20070816	US 2006-593129	20060918
US 7358400	B2	20080415		

PRIORITY APPLN. INFO.: JP 2004-104862 A 20040331
WO 2005-JP6407 W 20050325

OTHER SOURCE(S): MARPAT 143:386684
ED Entered STN: 14 Oct 2005
GI



I



II

AB A process for industrially advantageously and easily producing a cyclopropane monoacetal derivative represented by the general formula I [R1-R6 = independently H, (un)substituted saturated hydrocarbon, aryl, alkenyl or aralkyl; R8, R9 = independently (un)substituted saturated hydrocarbon, aryl or aralkyl] through a small number of steps, characterized by reacting a halogenated unsatd. carbonyl compound represented by the general formula II [R1-R6 and R8 are defined as above; X = halo] with an alcoholate. For example, reaction of tri-Et orthoformate with 2,3-dihydrofuran, and followed by chlorination with thionyl chloride, gave 4-chloro-2-ethoxymethylidenebutanal (III). Reaction of III with sodium ethoxide provided 1-(diethoxymethyl)cyclopropanecarbaldehyde.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 1 OF 1 CASREACT COPYRIGHT 2009 ACS on STN
AN 136:247742 CASREACT Full-text
TI Process for the preparation of pregnane derivatives
IN Nakazawa, Makoto
PA Kuraray Co., Ltd., Japan
SO PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07J005-00
CC 32-5 (Steroids)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002020552	A1	20020314	WO 2001-JP7639	20010904
	W: CA, CN, HU, IN, MX, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	JP 2002201199	A	20020716	JP 2001-261586	20010830
	CA 2416850	A1	20030120	CA 2001-2416850	20010904
	EP 1325928	A1	20030709	EP 2001-961343	20010904
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
	US 20030181742	A1	20030925	US 2003-363405	20030304
PRAI	JP 2000-273387	20000908			
	WO 2001-JP7639	20010904			

OS MARPAT 136:247742
GI

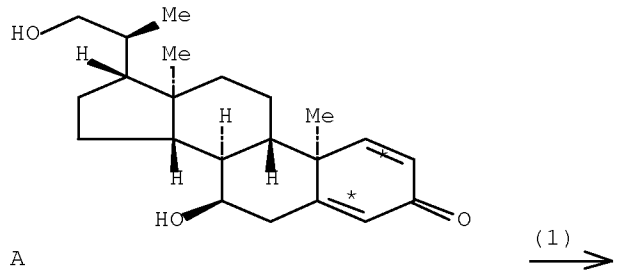
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A process for the preparation of pregnane derivs. [I; R1 = H; R2 = protecting group; R3, R4 independently = alkyl, aryl, alkenyl, alkynyl; R3R4 = alkylene] which comprises reacting a compound II with an alkali metal or an alkaline earth metal in the presence of ammonia or an amine to obtain a compound III (R1 = H; R2 = H), protecting the hydroxyl groups of the compound III to obtain a compound III (R1 = protecting group; R2 = protecting group) protecting the compound III (R1 = protecting group; R2 = protecting group) at the 3-position to obtain a compound I (R1 = protecting group; R2 = protecting group; R3, R4 independently = alkyl, aryl, alkenyl, alkynyl; R3R4 = alkylene), and subjecting the compound I (R1 = protecting group; R2 = protecting group; R3, R4 independently = alkyl, aryl, alkenyl, alkynyl; R3R4 = alkylene) to solvolysis to obtain a compound I (R1 = H; R2 = protecting group; R3, R4 independently = alkyl, aryl, alkenyl, alkynyl; R3R4 = alkylene) and compound III (R1 = H; R2 = H). Thus, the title compound I (R1 = H; R2 = C6H5CO; R3R4 = CH2CH2) was prepared effectively from (20S)-7-α-hydroxy-3-oxo-pregna-1,4-diene-20-carboxaldehyde and C6H5COCl via hydrogenation and ethylene glycol and C6H5COCl O-protection and was useful as intermediate for squalamine preparation

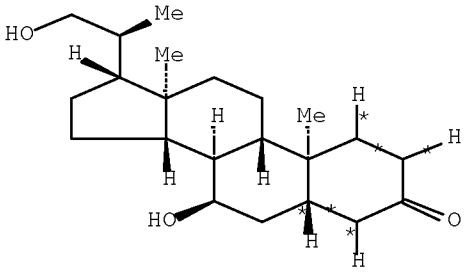
ST pregnane prepn redn hydrogenation solvolysis
IT Hydrogenation
Reduction
Solvolysis

(process for the preparation of pregnane derivs.)
IT 5132-07-0 7681-52-9
RL: RGT (Reagent); RACT (Reactant or reagent)
(compound for comparison in process for the preparation of pregnane derivs.)
IT 122197-36-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the preparation of pregnane derivs.)
IT 208833-68-5P 296768-82-6P 403854-15-9P 403854-16-0P 403854-17-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of pregnane derivs.)
IT 6192-52-5, p-Toluenesulfonic acid monohydrate
RL: RGT (Reagent); RACT (Reactant or reagent)
(process for the preparation of pregnane derivs.)
IT 208254-12-0P 301695-48-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of pregnane derivs.)
IT 107-21-1, Ethylene glycol, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(protecting process for the preparation of pregnane derivs.)
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; Bioorg Med Chem 2000, V8(8), P2059
(2) Anon; Chem Pharm Bull 1993, V41(4), P763
(3) Anon; Organic Letters 2000, V2(19), P2921
(4) Hoffmann La Roche F Und Co A G; EP 18515 A2 1980 CAPLUS
(5) Hoffmann La Roche F Und Co A G; US 4230625 A 1980 CAPLUS
(6) Hoffmann La Roche F Und Co A G; US 4301246 A 1980 CAPLUS
(7) Hoffmann La Roche F Und Co A G; JP 568399 A 1980
(8) Magainin Pharm Inc; JP 08507527 A 1994
(9) Magainin Pharm Inc; US 5637691 A 1994 CAPLUS
(10) Magainin Pharm Inc; EP 688333 A1 1994 CAPLUS
(11) Magainin Pharm Inc; WO 9420520 A1 1994 CAPLUS
(12) Magainin Pharm Inc; AU 9463974 A 1994 CAPLUS

RX(1) OF 35 ...A ===> B...



A (1) →



B
YIELD 65%

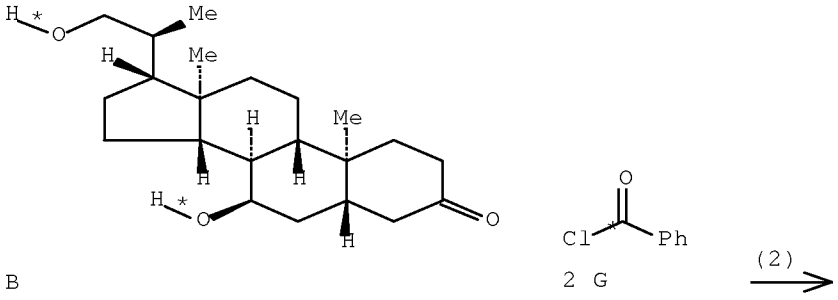
RX(1) RCT A 296768-82-6

STAGE(1)
SOL 109-99-9 THF

STAGE(2)
RGT C 7664-41-7 NH3, D 7439-93-2 Li
SOL 7732-18-5 Water

PRO B 301695-48-7
NTE -78°, under nitrogen

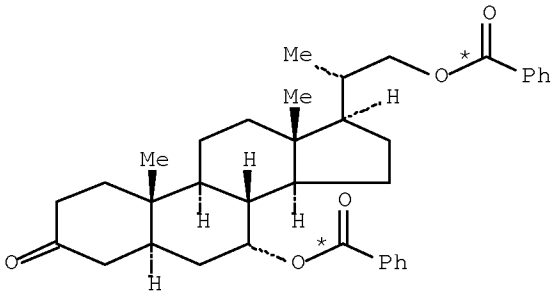
RX(2) OF 35 ...B + 2 G ===> H...



B

2 G

(2)



H
YIELD 90%

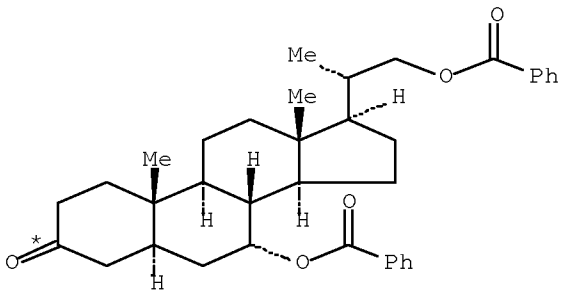
RX(2) RCT B 301695-48-7

STAGE(1)
RGT I 1122-58-3 4-DMAP, J 110-86-1 Pyridine
SOL 75-09-2 CH2Cl2

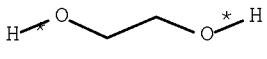
STAGE(2)
RCT G 98-88-4

PRO H 403854-15-9
NTE 0°, under nitrogen in first step, room temp. for 12 h in second step

RX(3) OF 35 ...H + L ===> M...

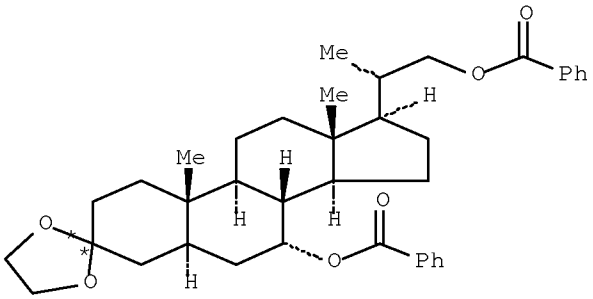


H



L

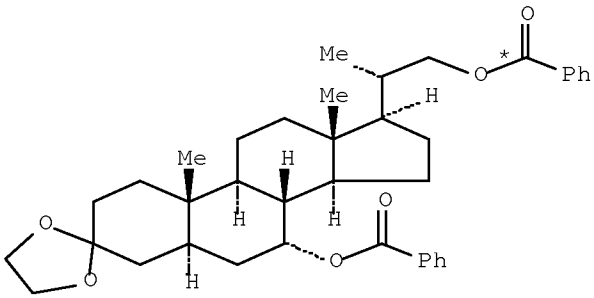
(3)



M
YIELD 97%

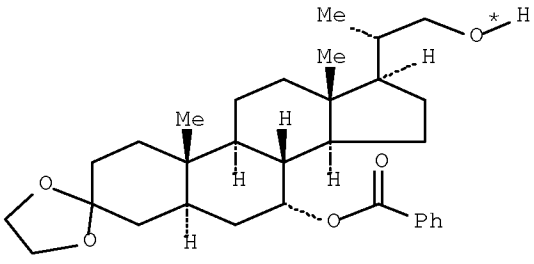
RX(3) RCT H 403854-15-9, L 107-21-1
       RGT N 104-15-4 TsOH
       PRO M 403854-16-0
       SOL 108-88-3 PhMe
       NTE reflux, 2 h

RX(4) OF 35 ...M ===> P...



M

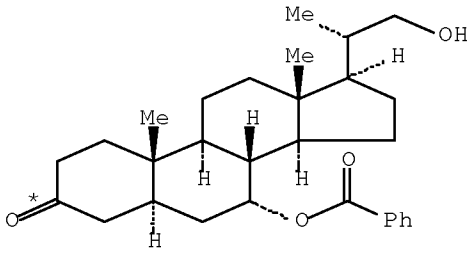
(4)



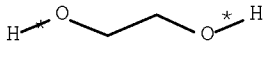
P
YIELD 86%

RX(4) RCT M 403854-16-0
RGT Q 1310-73-2 NaOH
PRO P 208833-68-5
SOL 67-56-1 MeOH, 109-99-9 THF
NTE room temp., 11 h

RX(5) OF 35 ...S + L ===> P...

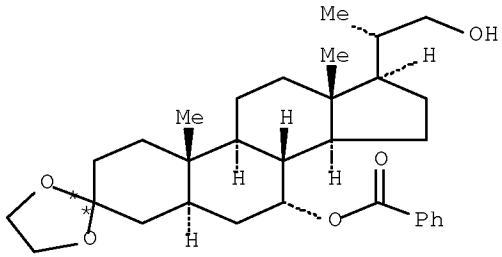


S



L

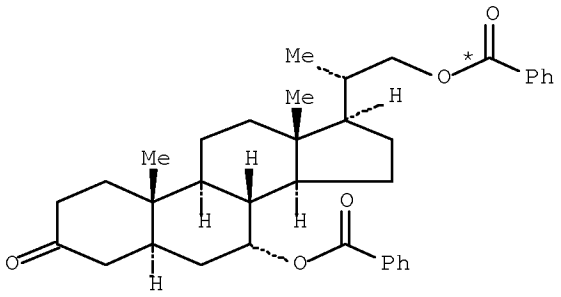
(5)



P
YIELD 28%

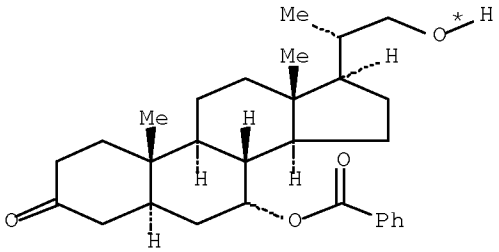
RX(5) RCT S 403854-17-1, L 107-21-1
RGT T 6192-52-5 p-MeC6H4SO3H.H20
PRO P 208833-68-5
SOL 108-88-3 PhMe
NTE reflux, 40 h

RX(6) OF 35 ...H ===> S...



H

(6)



S
YIELD 69%

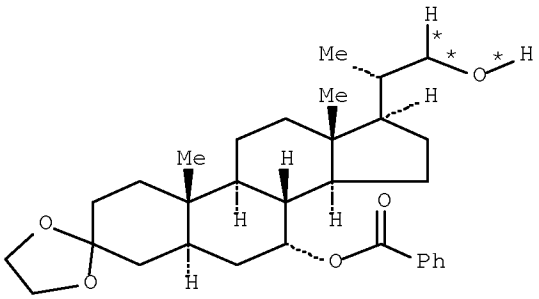
RX(6) RCT H 403854-15-9

STAGE(1)
SOL 109-99-9 THF

STAGE(2)
RGT U 497-19-8 Na2CO3, Q 1310-73-2 NaOH
SOL 7732-18-5 Water, 67-56-1 MeOH

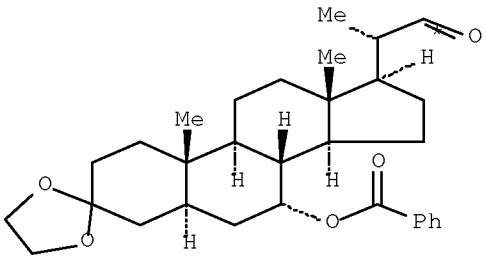
PRO S 403854-17-1
NTE 40°, 4 h

RX(7) OF 35 ...P ===> V



P

(7)



V
YIELD 79%

RX(7) RCT P 208833-68-5

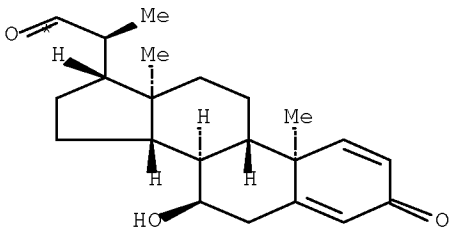
STAGE(1)
RGT W 5132-07-0 Piperidine, 2,2,6,6-tetramethyl-, 1-oxide
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT X 7758-02-3 KBr
SOL 7732-18-5 Water

STAGE(3)
RGT Y 7681-52-9 NaOCl, U 497-19-8 Na2CO3
SOL 7732-18-5 Water

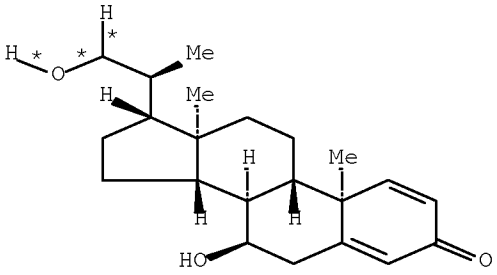
PRO V 208254-12-0
NTE 0°, 2 h

RX(8) OF 35 Z ===> A...



Z

(8)



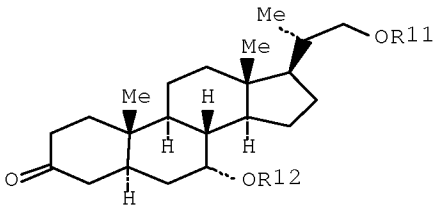
A
YIELD 93%

RX(8) RCT Z 122197-36-8
RGT AA 16940-66-2 NaBH4
PRO A 296768-82-6
SOL 64-17-5 EtOH
NTE 0°

L8 ANSWER 1 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1196549 HCAPLUS Full-text
DOCUMENT NUMBER: 143:440617
TITLE: Preparation of 5-pregnanones as intermediates for squalamine
INVENTOR(S): Koyakumaru, Kenichi
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005314405	A	20051110	JP 2005-100945	20050331 <--
PRIORITY APPLN. INFO.:			JP 2004-108460 A	20040331 <--

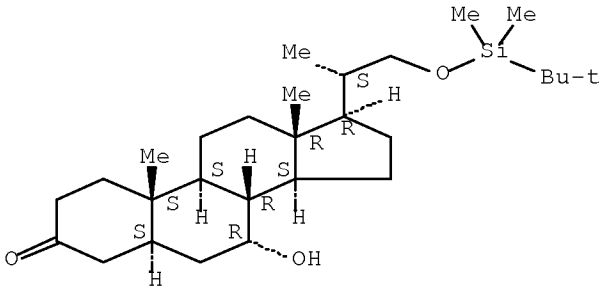
OTHER SOURCE(S): MARPAT 143:440617
ED Entered STN: 10 Nov 2005
GI



I

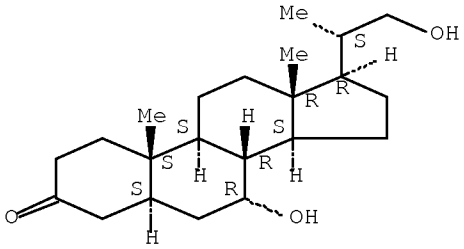
AB 5-Pregnanones I (R11, R12 = H, protecting group) are prepared by selective hydrogenation of C-C double bond of their corresponding 5-pregn-1-en-3-ones. Thus, (20S)-7α,21-dihydroxy-20-methyl-5α- pregn-1-en-3-one was hydrogenated over Pd/C at 50° for 22 h in THF to give 95% (20S)-7α,21-dihydroxy-20-methyl-5α-pregnan-3-one.
IT 303178-20-3P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pregnanones as intermediates for squalamine from pregnenones)
RN 303178-20-3 HCAPLUS
CN Pregnan-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



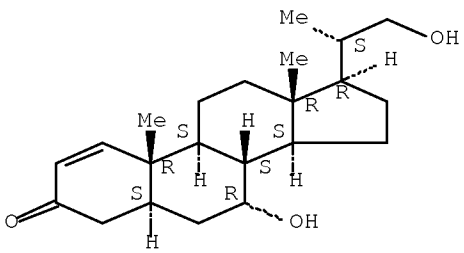
IT 301695-48-7P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of pregnanones as intermediates for squalamine from pregnenones)
RN 301695-48-7 HCAPLUS
CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



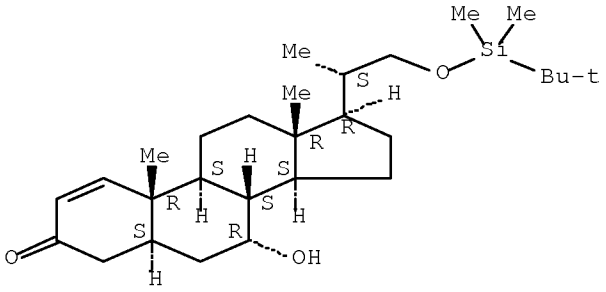
IT 866488-96-2P 866562-46-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pregnanones as intermediates for squalamine from pregnenones)
RN 866488-96-2 HCAPLUS
CN Pregn-1-en-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 866562-46-1 HCAPLUS
CN Pregn-1-en-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

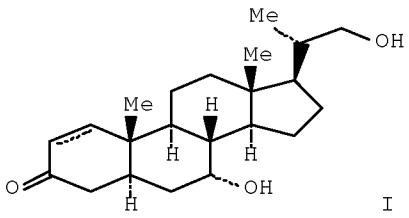
Absolute stereochemistry.



L8 ANSWER 2 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1125857 HCAPLUS Full-text
DOCUMENT NUMBER: 143:387238
TITLE: Preparation of 5α-pregnane derivative as intermediate for squalamine
INVENTOR(S): Nakasawa, Makoto; Koyakumaru, Kenichi
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005289901	A	20051020	JP 2004-108416	20040331 <--

PRIORITY APPLN. INFO.: JP 2004-108416 20040331 <--
ED Entered STN: 20 Oct 2005
GI



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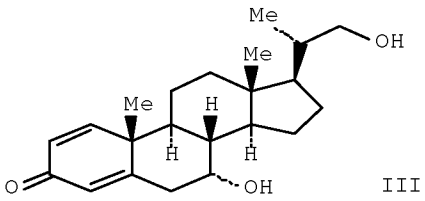


III

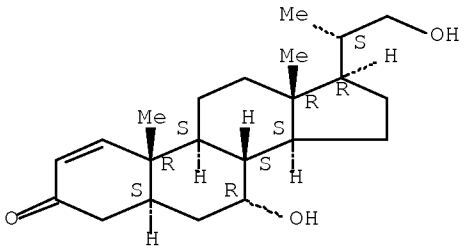
AB Title derivative I (the broken line is none: II) is prepared by treatment of pregnadienone derivative III with alkali metals or alkaline earth metals in the presence of amines and/or ammonia, followed by reduction of resulting mixture of I (the broken line is bond: IV) and II. Thus, hydrogenation of III with Li and ammonia at -40° in THF gave II-IV mixture, which was hydrogenated over Pd/C to give II.

IT 866488-96-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 5α-pregnane derivative as intermediate for squalamine from pregnadienone derivative)

RN 866488-96-2 HCAPLUS

CN Pregn-1-en-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

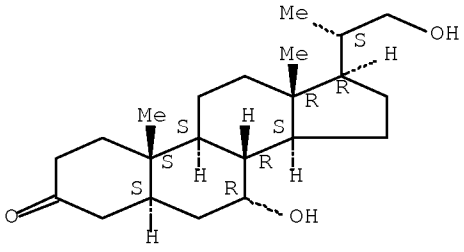


IT 301695-48-7P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 5α-pregnane derivative as intermediate for squalamine from pregnadienone derivative)

RN 301695-48-7 HCAPLUS

CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 3 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1106865 HCAPLUS Full-text

DOCUMENT NUMBER: 143:387237

TITLE: Process for the preparation of 5α-pregnane derivative via reduction of carbon-carbon double bond

in pregn-4-en-3-one compound

INVENTOR(S): Sugioka, Takashi; Ohzono, Shigeo; Koyakumaru, Kenichi; Nakagawa, Naoshi

PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2005095434	A1	20051013	WO 2005-JP6828		20050331	<--
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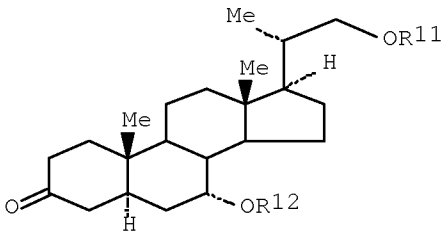
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG						
EP 1743902	A1	20070117	EP 2005-728917		20050331	<--
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR						
CN 1934124	A	20070321	CN 2005-80009530		20050331	<--
US 20070149494	A1	20070628	US 2006-594164		20060926	<--
IN 2006CN03994	A	20070706	IN 2006-CN3994		20061031	<--
PRIORITY APPLN. INFO.:			JP 2004-108419	A	20040331	<--
			WO 2005-JP6828	W	20050331	<--

OTHER SOURCE(S): MARPAT 143:387237

ED Entered STN: 14 Oct 2005

GI



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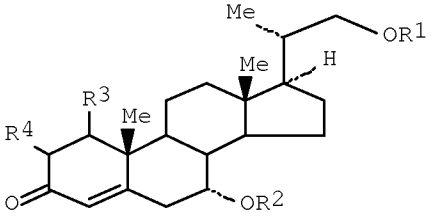


II

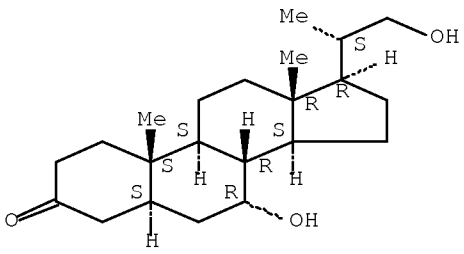
AB A process for the preparation of compound I [R11, R12 = H, protecting group of hydroxy], characterized by reduction a pregnane derivative II [R1 = protecting group of hydroxy; R2 = H, protecting group of hydroxy; R3 and R4 represent hydrogen atoms or combine together to form a bond.] with alkali metals or alkaline earth metals in the presence of a proton donor, amine and/or ammonia, was disclosed. For example, to a solution of (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methylpregn-4-en-3- one (5.00 g) and tert-butanol (1.78 g) in THF (100 mL) was added liquid ammonia (100 mL) at -50 °C. Then, Li metal (0.17 g) was added, while maintaining the reaction temperature between -50 and -40 °C, the reaction was stirred -40 °C for 3 h. The resulting reaction was treated with ammonium sulfate (1.59 g) followed by removal of ammonia, aqueous work-up and silica-gel purification to give (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methyl-5α- pregn-3-one in 96% yield. Of note compds. I are useful synthetic intermediates for the preparation of squalamine.

IT 301695-48-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (20S)-7α,21-dihydroxy-20-methyl-5α-pregn-3-one via reduction and desilylation)

RN 301695-48-7 HCAPLUS

CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

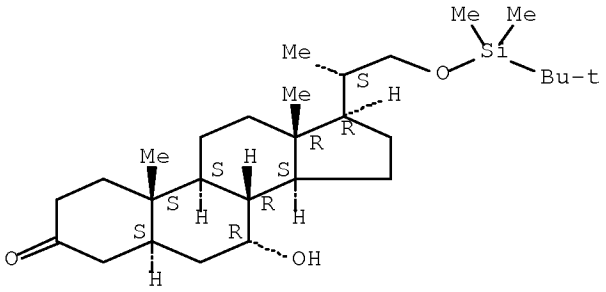


IT 303178-20-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 5α-pregn-3-one compound from pregn-4-en-3-one via reduction using Li metal and ammonia)

RN 303178-20-3 HCAPLUS

CN Pregnan-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



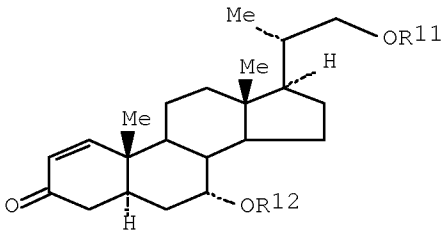
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103799 HCAPLUS Full-text
DOCUMENT NUMBER: 143:387235
TITLE: Process for the preparation of 5α-pregn-1-en-3-one derivative via reduction of carbon-carbon double bond in pregn-1,4-dien-3-one compound
INVENTOR(S): Koyakumaru, Kenichi
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095433	A1	20051013	WO 2005-JP6824	20050331 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 2004-108451 A 20040331 <--
OTHER SOURCE(S): MARPAT 143:387235
ED Entered STN: 14 Oct 2005
GI



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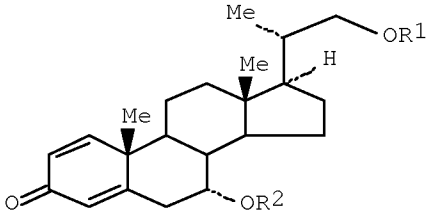


II

AB A process for the preparation of compds. I [R11, R12 = H, protecting group of hydroxy] from compds. II [R1 = protecting group of hydroxy; R2 = H, protecting group of hydroxy] using alkali metals or alkaline earth metals in the presence of a proton donor, amine and/or ammonia, was disclosed. For example, to a solution of (20S)-21-tert-butyldimethylsilyloxy-7α- hydroxy-20-methylpregn-1,4-dien-3-one (10.00 g) and tert-butanol (3.23 g) in THF (170 mL) was added liquid ammonia (170 mL) at -50 °C. Then, Li metal (0.32 g) was added, while maintaining reaction temperature between -50 to -40 °C, the reaction was stirred at -40 °C for 2 h. The resulting mixture was treated with ammonium acetate (1.17 g) followed by removal of ammonia, aqueous work-up and silica-gel purification to give (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methyl-5α- pregn-1-en-3-one in 78% yield. Of note, compds. I are useful synthetic intermediates for the preparation of squalamine.

IT 866488-96-2P

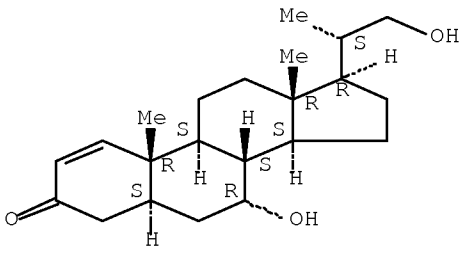
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(desilylation of (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methylpregn-1-en-3-one)

RN 866488-96-2 HCAPLUS

CN Pregn-1-en-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



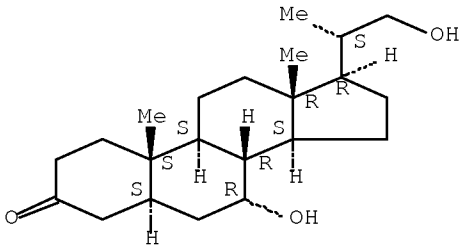
IT 301695-48-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (20S)-7α,21-dihydroxy-20-methyl-5α-pregn-3-one via Pd/C catalyzed hydrogenation)

RN 301695-48-7 HCAPLUS

CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



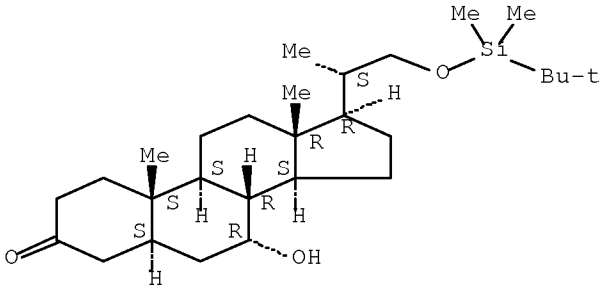
IT 303178-20-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 21-silyloxy-5α-pregn-3-one compound from 21-silyloxy-5α-pregn-1-en-3-one derivative via Pd/C catalyzed hydrogenation)

RN 303178-20-3 HCAPLUS

CN Pregnan-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



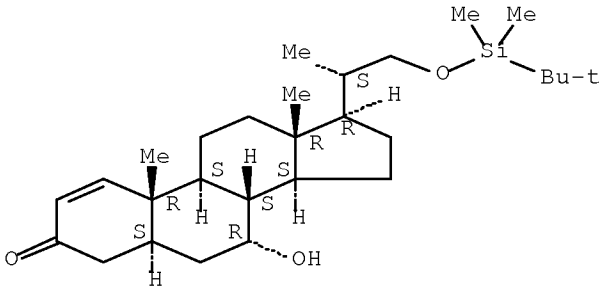
IT 866562-46-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pregn-1-en-3-one derivs. from pregn-1,4-dien-3-one compound via reduction using Li metal and ammonia)

RN 866562-46-1 HCAPLUS

CN Pregn-1-en-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103798 HCAPLUS Full-text
DOCUMENT NUMBER: 143:387234
TITLE: Process for the preparation of 5α-pregnane derivative via reduction of carbon-carbon double bond in 5α-pregn-1-en-3-one
INVENTOR(S): Koyakumaru, Kenichi
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005095432	A1	20051013	WO 2005-JP6819		20050331 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
EP 1731526	A1	20061213	EP 2005-728912		20050331 <--
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR					
CN 1938331	A	20070328	CN 2005-80010329		20050331 <--
US 20070203106	A1	20070830	US 2006-594401		20060926 <--
IN 2006CN04001	A	20070629	IN 2006-CN4001		20061031 <--
PRIORITY APPLN. INFO.:			JP 2004-108443	A	20040331 <--
			WO 2005-JP6819	W	20050331 <--

OTHER SOURCE(S): MARPAT 143:387234
ED Entered STN: 14 Oct 2005
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

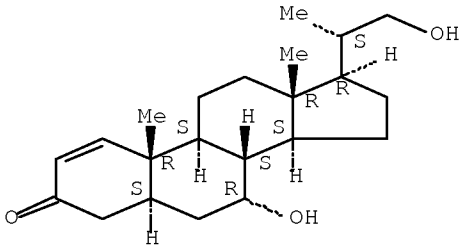
AB Process for the preparation of compound I [R11, R12 = H, protecting group of hydroxy], characterized by selectively reducing a carbon-carbon double bond in a mixture of 5α-pregnane derivs. II [R1, R2 = H, protecting group of hydroxy] and III [R1, R2 = same as above], was disclosed. For example, a mixture of (20S)-7α,21-dihydroxy-20-methyl-5α-pregn-3- one (2.76 g) and (20S)-7α,21-dihydroxy-20-methyl-5α-pregn-1-en- 3-one (0.46 g) in THF was hydrogenated in the presence of 10% Pd/C (50 mg) under H2 atmosphere at 50 °C for 5 h to give (20S)-7α,21-dihydroxy-20-methyl-5α-pregn-3-one (3.06 g). Of note, compds. I are useful synthetic intermediates for the preparation of squalamine.

IT 866488-96-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(desilylation of a mixture of (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methyl-5α-pregn-1-en-3-one and (20S)-21-tert-Butyldimethylsilyloxy-7α-hydroxy-20-methyl-5α-pregn-3-one)

RN 866488-96-2 HCAPLUS

CN Pregn-1-en-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

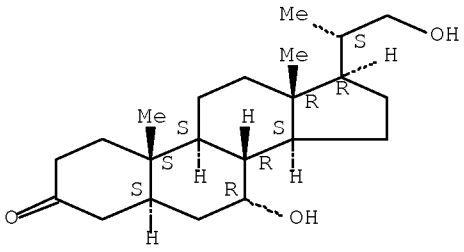


IT 301695-48-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (20S)-7α,21-dihydroxy-20-methyl-5α-pregn-3-one via desilylation of silylated pregn-one derivs. or hydrogenation of pregnenone derivs.)

RN 301695-48-7 HCAPLUS

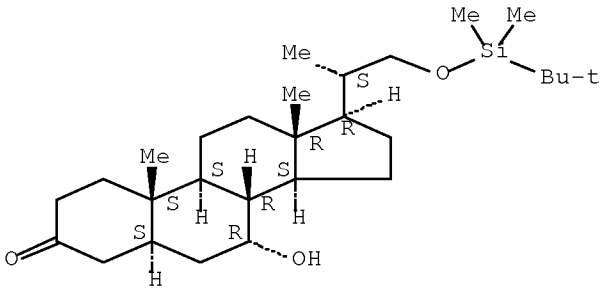
CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



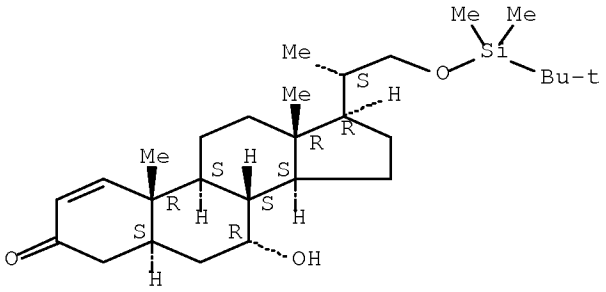
IT 303178-20-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reduction of (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methylpregn-1,4-dien-3-one using Li metal and ammonia)
RN 303178-20-3 HCAPLUS
CN Pregnan-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 866562-46-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reduction of (20S)-7α,21-dihydroxy-20-methylpregn-1,4-dien-3-one using Li metal and ammonia)
RN 866562-46-1 HCAPLUS
CN Pregn-1-en-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

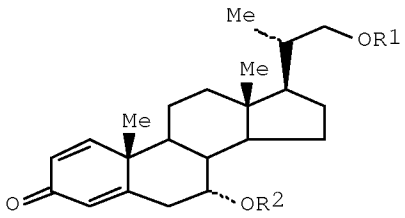


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103797 HCAPLUS Full-text
DOCUMENT NUMBER: 143:387233
TITLE: Method for producing 5α-pregnane derivative
INVENTOR(S): Koyakumaru, Kenichi; Sugioka, Takashi; Ohzono, Shigeo; Nakagawa, Naoshi
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095431	A1	20051013	WO 2005-JP6818	20050331 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1938330	A	20070328	CN 2005-80010110	20050331 <--
EP 1767540	A1	20070328	EP 2005-728889	20050331 <--
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
US 20070197490	A1	20070823	US 2006-594163	20060926 <--
IN 2006CN03996	A	20070706	IN 2006-CN3996	20061031 <--
PRIORITY APPLN. INFO.:			JP 2004-108434 A	20040331 <--
			WO 2005-JP6818 W	20050331 <--

OTHER SOURCE(S): MARPAT 143:387233
ED Entered STN: 14 Oct 2005
GI



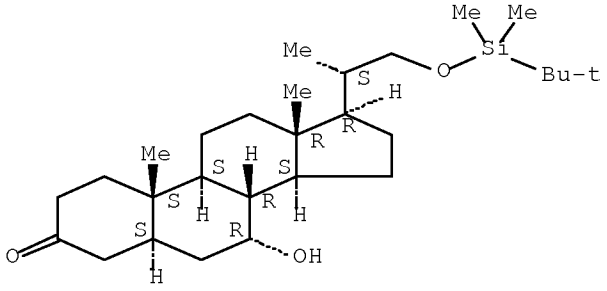
I

AB 5α-Pregna-3-one derivs. and 5α-pregna-1-en-3-one derivs. are prepared by reacting a pregnane derivative represented by the general formula I [R1 = OH-protecting group; R2 = H, OH-protecting group] with a metal selected from alkali metals and alkaline earth metals in the presence of a proton donor, an amine and/or ammonia. The title compds. are intermediates for squalamine. Thus, (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20-methyl-5α- pregna-3-one and (20S)-21-tert-butyldimethylsilyloxy-7α-hydroxy-20- methyl-5α-pregna-1-en-3-one were prepared by the title method.

IT 303178-20-3P 866562-46-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(method for producing 5α-pregnane derivs. by reduction of methylpregna-1,4-dien-3-one derivs.)

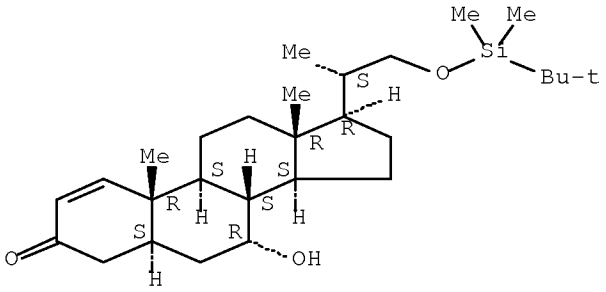
RN 303178-20-3 HCAPLUS
CN Pregnan-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



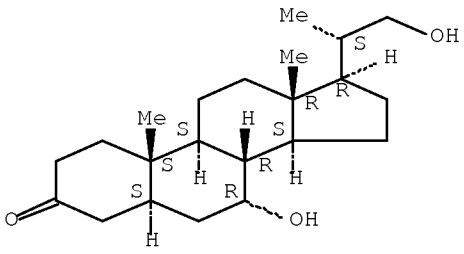
RN 866562-46-1 HCAPLUS
CN Pregn-1-en-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



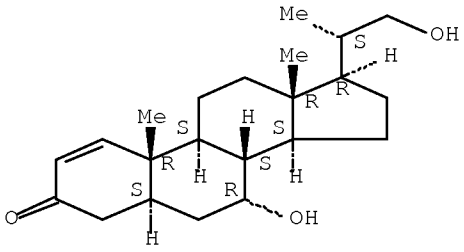
IT 301695-48-7P 866488-96-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(method for producing 5α-pregnane derivs. by reduction of methylpregna-1,4-dien-3-one derivs.)
RN 301695-48-7 HCAPLUS
CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 866488-96-2 HCAPLUS
CN Pregn-1-en-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



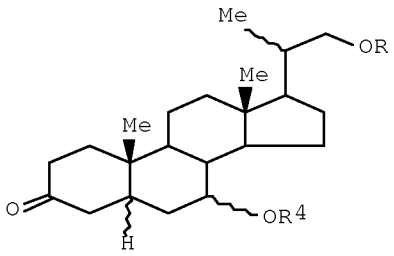
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:491250 HCAPLUS Full-text
DOCUMENT NUMBER: 139:69426
TITLE: Process for producing pregnane derivative
INVENTOR(S): Nakazawa, Makoto; Ohzono, Shigeo
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051904	A1	20030626	WO 2002-JP11547	20021106 <--
W: CA, CN, HU, IN, MX, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR				
JP 2003246790	A	20030902	JP 2002-322581	20021106 <--
PRIORITY APPLN. INFO.:			JP 2001-386808 A	20011219 <--

OTHER SOURCE(S): MARPAT 139:69426
ED Entered STN: 27 Jun 2003
GI



I

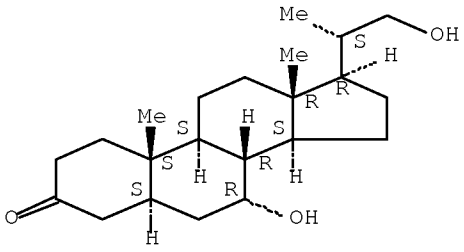
AB This document discloses a process for producing a 21-hydroxypregnane derivative represented by the general formula I [R = H; R4 represents a hydroxy-protecting group.] characterized by protecting the 7-position hydroxy group of a compound represented by the formula I [R = SiR1R2R3; R1, R2, and R3 each independently represents optionally substituted alkyl, alkenyl, alkynyl, aryl, or aralkyl; and R4 = H] and subsequently eliminating the 21-position protective silyl group. An intermediate for squalamine can be efficiently produced by the title process.

IT 301695-48-7P 303178-20-3P 550372-80-0P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for producing pregnane derivative)

RN 301695-48-7 HCAPLUS

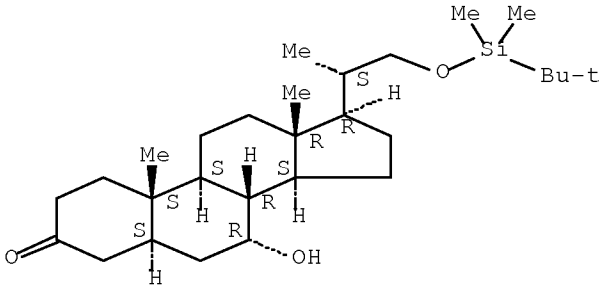
CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



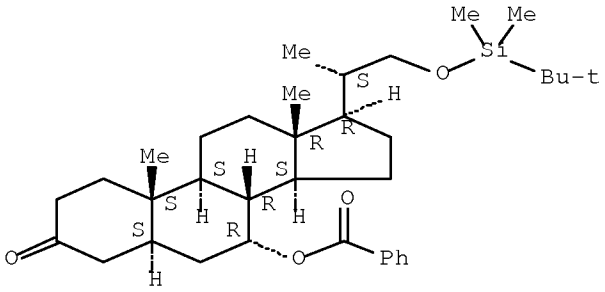
RN 303178-20-3 HCAPLUS
CN Pregnan-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 550372-80-0 HCAPLUS
CN Pregnan-3-one, 7-(benzoyloxy)-21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-20-methyl-, (5α,7α,21S)- (9CI) (CA INDEX NAME)

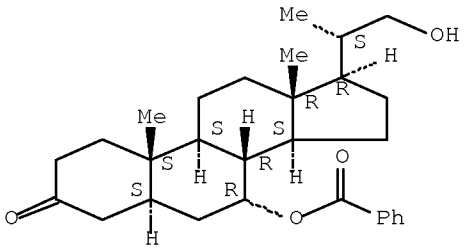
Absolute stereochemistry.



IT 403854-17-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for producing pregnane derivative)
RN 403854-17-1 HCAPLUS
CN Pregnan-3-one, 7-(benzoyloxy)-21-hydroxy-20-methyl-,

(5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:185147 HCAPLUS Full-text
DOCUMENT NUMBER: 136:247742
TITLE: Process for the preparation of pregnane derivatives
INVENTOR(S): Nakazawa, Makoto
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002020552	A1	20020314	WO 2001-JP7639		20010904 <--
W: CA, CN, HU, IN, MX, US					
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR					
JP 2002201199	A	20020716	JP 2001-261586		20010830 <--
CA 2416850	A1	20030120	CA 2001-2416850		20010904 <--
EP 1325928	A1	20030709	EP 2001-961343		20010904 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR					
US 20030181742	A1	20030925	US 2003-363405		20030304 <--
PRIORITY APPLN. INFO.:			JP 2000-273387	A	20000908 <--
			WO 2001-JP7639	W	20010904 <--

OTHER SOURCE(S): CASREACT 136:247742; MARPAT 136:247742
ED Entered STN: 15 Mar 2002
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

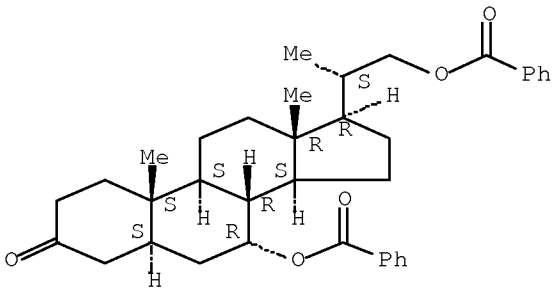
AB A process for the preparation of pregnane derivs. [I; R1 = H; R2 = protecting group; R3, R4 independently = alkyl, aryl, alkenyl, alkynyl; R3R4 = alkylene] which comprises reacting a compound II with an alkali metal or an alkaline earth metal in the presence of ammonia or an amine to obtain a compound III

(R1 = H; R2 = H), protecting the hydroxyl groups of the compound III to obtain a compound III (R1 = protecting group; R2 = protecting group) protecting the compound III (R1 = protecting group; R2 = protecting group) at the 3-position to obtain a compound I (R1 = protecting group; R2 = protecting group; R3, R4 independently = alkyl, aryl, alkenyl, alkynyl; R3R4 = alkylene), and subjecting the compound I (R1 = protecting group; R2 = protecting group; R3, R4 independently = alkyl, aryl, alkenyl, alkynyl; R3R4 = alkylene) to solvolysis to obtain a compound I (R1 = H; R2 = protecting group; R3, R4 independently = alkyl, aryl, alkenyl, alkynyl; R3R4 = alkylene) and compound III (R1 = H; R2 = H). Thus, the title compound I (R1 = H; R2 = C6H5CO; R3R4 = CH2CH2) was prepared effectively from (20S)-7-α-hydroxy-3-oxo-pregna-1,4-diene-20-carboxaldehyde and C6H5COCl via hydrogenation and ethylene glycol and C6H5COCl O-protection and was useful as intermediate for squalamine preparation

IT 403854-15-9P 403854-17-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of pregnane derivs.)

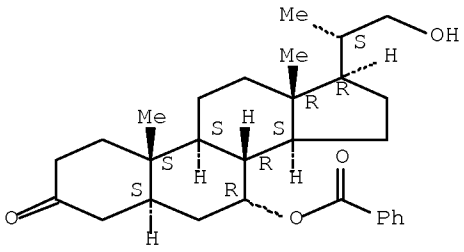
RN 403854-15-9 HCAPLUS
CN Pregnan-3-one, 7,21-bis(benzoyloxy)-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 403854-17-1 HCAPLUS
CN Pregnan-3-one, 7-(benzoyloxy)-21-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

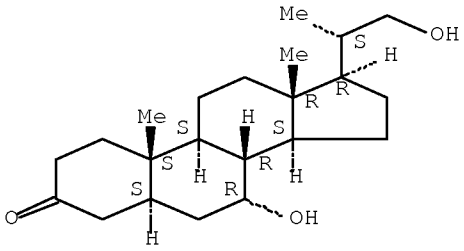
Absolute stereochemistry.



IT 301695-48-7P
RL: SPN (Synthetic preparation); PREP (Preparation)

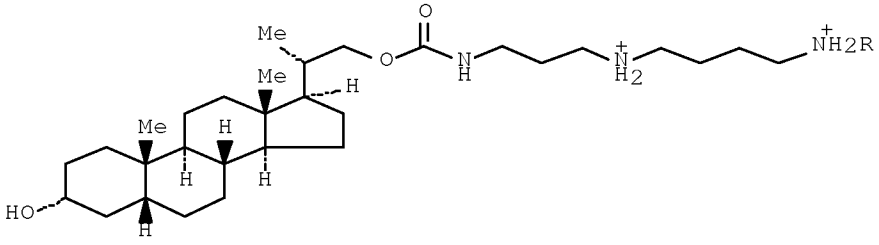
(process for the preparation of pregnane derivs.)
RN 301695-48-7 HCAPLUS
CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:872204 HCAPLUS Full-text
DOCUMENT NUMBER: 136:167554
TITLE: Synthesis and antimicrobial activity of new 3α-Hydroxy-23,24-bisnorcholane polyamine carbamates
AUTHOR(S): Kim, Hong-Seok; Kwon, Kyung-Chan; Kim, Ki Soo; Lee, Cheol Hae
CORPORATE SOURCE: Department of Industrial Chemistry, Kyungpook National University, Taegu, 702-701, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(23), 3065-3068
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:167554
ED Entered STN: 04 Dec 2001
GI



I

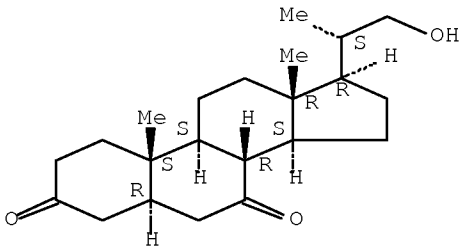
AB 3α-Hydroxy-23,24-bisnorcholane spermidine and spermine carbamates, e.g. I.2Cl-, have been synthesized and their antimicrobial and hemolytic activities were

evaluated. They exhibited excellent in vitro activities especially against methicillin-resistant Staphylococcus aureus.

IT 398138-67-5 781657-55-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bisnorcholane polyamine carbamates and antimicrobial activity against methicillin-resistant Staphylococcus aureus)

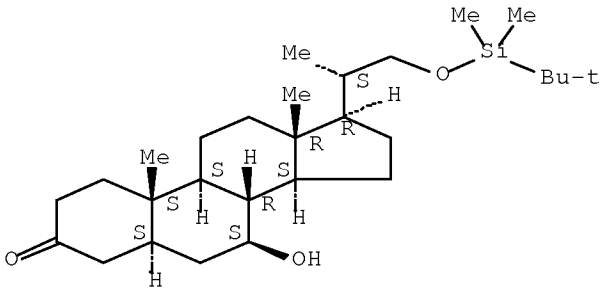
RN 398138-67-5 HCAPLUS
CN Pregnane-3,7-dione, 21-hydroxy-20-methyl-, (5α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 781657-55-4 HCAPLUS
CN Pregnan-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7β,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



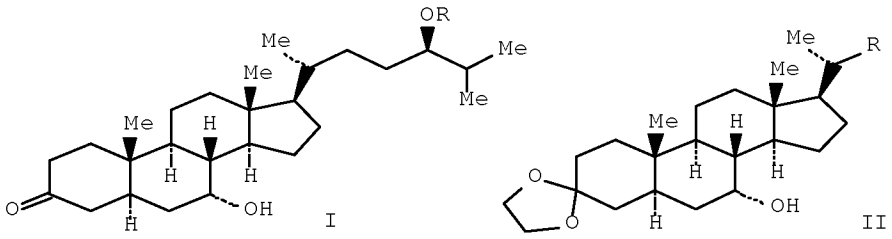
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 10 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:780935 HCAPLUS Full-text
DOCUMENT NUMBER: 135:318612
TITLE: A process for the preparation of 7α-hydroxy 3-aminosubstituted sterols using intermediates with an unprotected 7α-hydroxy group
INVENTOR(S): Kinney, William A.; Zhang, Xuehai; Michalak, Ronald
PATENT ASSIGNEE(S): Genaera Corporation, USA
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2001079255	A1	20011025	WO 2001-US12004		20010412	<--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW						
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
CA 2406847	A1	20011025	CA 2001-2406847		20010412	<--
EP 1274718	A1	20030115	EP 2001-926924		20010412	<--
EP 1274718	B1	20061018				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR						
JP 2003531148	T	20031021	JP 2001-576852		20010412	<--
AT 342912	T	20061115	AT 2001-926924		20010412	<--
AU 2001253427	B2	20070208	AU 2001-253427		20010412	<--
ES 2273831	T3	20070516	ES 2001-926924		20010412	<--
US 20030171576	A1	20030911	US 2002-268660		20021011	<--
US 6933383	B2	20050823				
US 20050187202	A1	20050825	US 2005-83961		20050321	<--
PRIORITY APPLN. INFO.:			US 2000-196646P	P	20000412	<--
			WO 2001-US12004	W	20010412	<--
			US 2002-268660	A3	20021011	<--

OTHER SOURCE(S): CASREACT 135:318612; MARPAT 135:318612
ED Entered STN: 26 Oct 2001
GI



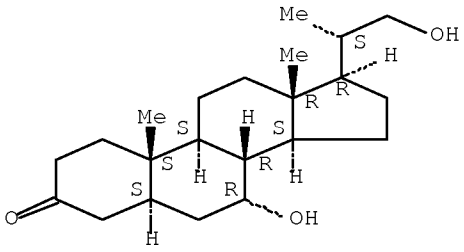
AB An efficient method for the synthesis of aminosterol compds. such as squalamine and compound 1436 is described. A method of the invention provides for regioselective oxidation and regioselective sulfonation of a fused ring system. The fused ring base can be, for example, a steroid ring base. The aminosterol compds. are effective as, among others, antibiotics, antiangiogenic agents and NHE3 inhibitors. Thus, squalamine and compound 1436 intermediate I (R = SO3H) was prepared by the regioselective oxidation of II (R = CH2OH) with NaOCl and TEMPO to give II (R = CHO), and regioselective sulfonation of I (R = H).
IT 301695-48-7P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 7α-hydroxy-3-amino-substituted steroids via regioselective oxidation and sulfonation)

RN 301695-48-7 HCAPLUS

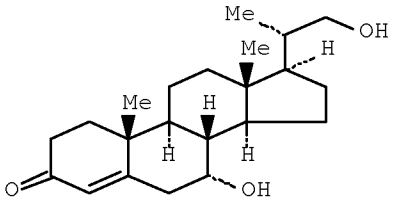
CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

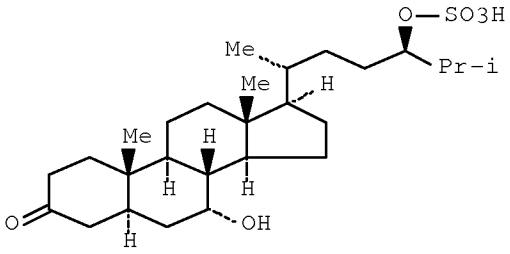


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:605979 HCAPLUS Full-text
DOCUMENT NUMBER: 133:310055
TITLE: A Short Formal Synthesis of Squalamine from a Microbial Metabolite
AUTHOR(S): Kinney, William A.; Zhang, Xuehai; Williams, Jon I.; Johnston, Sean; Michalak, Ronald S.; Deshpande, Milind; Dostal, Larry; Rosazza, John P. N.
CORPORATE SOURCE: Magainin Pharmaceuticals Inc., Plymouth Meeting, PA, 19462, USA
SOURCE: Organic Letters (2000), 2(19), 2921-2922
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:310055
ED Entered STN: 31 Aug 2000
GI



I



II

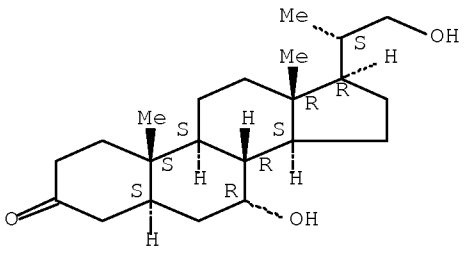
AB Formal synthesis of squalamine is described, utilizing the biotransformation product I, which is available in one step from com. available 3-keto-23,24-bisnorchol-4-en-22-ol. Regioselective C-22 oxidation and C-24 sulfation of the corresponding alcs. in the presence of a free C-7 alc. make for an efficient preparation of squalamine intermediate II.

IT 301695-48-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(formal synthesis of squalamine from a microbial metabolite)

RN 301695-48-7 HCAPLUS

CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

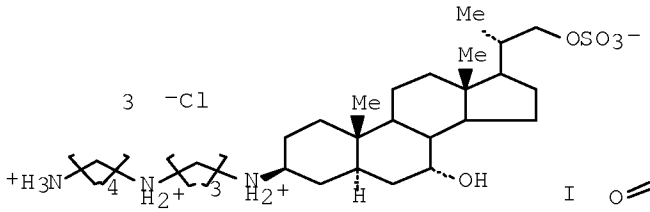
Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:564499 HCAPLUS Full-text
DOCUMENT NUMBER: 133:335386
TITLE: Synthesis and antimicrobial activity of squalamine analogue
AUTHOR(S): Kim, H.-S.; Choi, B.-S.; Kwon, K.-C.; Lee, S.-O.;

Kwak, H. J.; Lee, C. H.
CORPORATE SOURCE: Department of Industrial Chemistry, Kyungpook National University, Taegu, 702-701, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(8), 2059-2065
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:335386
ED Entered STN: 16 Aug 2000
GI



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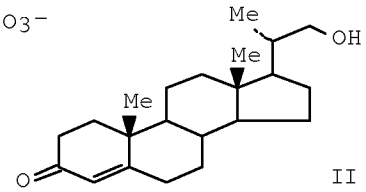
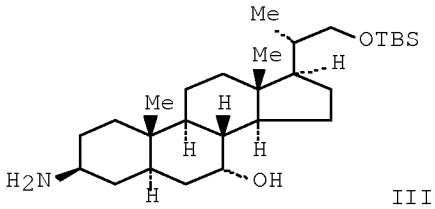
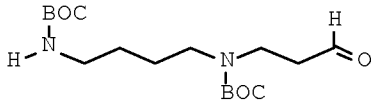


II



III



IV

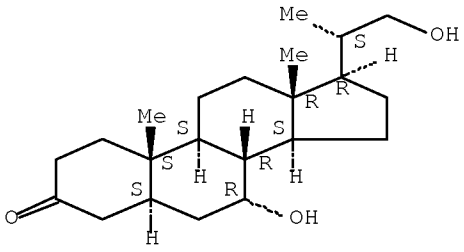
AB Synthesis and antimicrobial activity of squalamine analog (I) are reported. The synthesis of I was accomplished from bisnoralc. (II). The spermidine moiety was introduced via reductive amination of an appropriately functionalized 3β-aminosterol (III) with spermidinyl aldehyde (IV) utilizing sodium triacetoxyborohydride as the reducing agent. I shows weaker antimicrobial activity than squalamine.

IT 301695-48-7P 303178-20-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antimicrobial activity of squalamine analog)

RN 301695-48-7 HCAPLUS

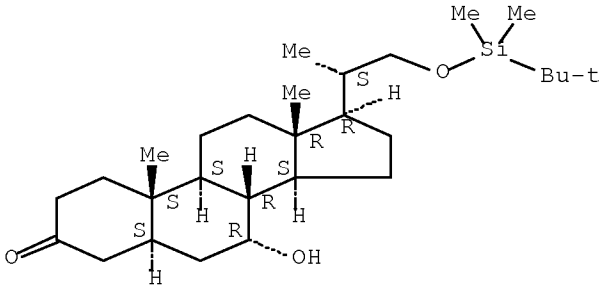
CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 303178-20-3 HCAPLUS
CN Pregnan-3-one, 21-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-hydroxy-20-methyl-, (5α,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1997:540987 HCAPLUS Full-text
DOCUMENT NUMBER: 127:229207
ORIGINAL REFERENCE NO.: 127:44531a,44534a
TITLE: Effect of side chain length on biotransformation, hepatic transport, and choleretic properties of chenodeoxycholyl homologs in the rodent: studies with dinorchenodeoxycholic acid, norchenodeoxycholic acid, and chenodeoxycholic acid
AUTHOR(S): Yeh, Hong-Zen; Schteingart, Claudio D.; Hagey, Lee R.; Ton-Nu, Huong-Thu; Bolder, Ulrich; Gavrilkina, Miriam A.; Steinbach, Joseph H.; Hofmann, Alan F.
CORPORATE SOURCE: div. Gastroenterol., Dep. Med., Univ. California San Diego, San Diego, CA, USA
SOURCE: Hepatology (Philadelphia) (1997), 26(2), 374-385
CODEN: HPTLD9; ISSN: 0270-9139
PUBLISHER: Saunders
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 25 Aug 1997
AB To assess the effect of side chain length on the metabolism and physiol. effects of homologs of chenodeoxycholic acid (CDCA), dinorCDCA, the C22 homolog, was synthesized and its hepatic biotransformation, transport

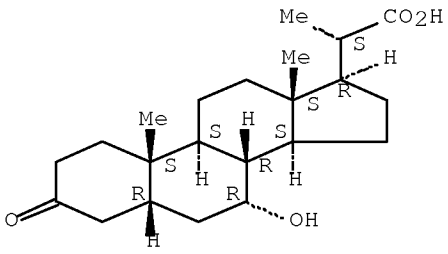
kinetics, and choleretic properties were defined in rat and hamster biliary fistula and in isolated perfused rat liver. Results were compared with those of norCDCA, the C23 homolog, and of CDCA, the natural C24 homolog. In the rat, dinorCDCA was secreted mostly in unconjugated form (the majority as dinor-α-muricholic acid); the remainder was glucuronidated. In the hamster, glucuronidation was greater, and the unconjugated fraction contained equal parts of dinor CDCA and 5β-hydroxy-dinorCDCA. NorCDCA was glucuronidated extensively (70%, rat; 40%, hamster). CDCA, in contrast, was efficiently amidated with taurine or glycine. In the perfused liver, the initial uptake rate of all three homologs was identical; later, regurgitation and/or cholehepatic shunting of dinor-CDCA and norCDCA, but not of CDCA, occurred. In rats and hamsters with biliary fistulas, dinorCDCA and norCDCA, but not CDCA, induced a bicarbonate-rich hypercholeresis of canalicular origin. Hypercholeresis was not induced by the taurine conjugate of dinorCDCA. Hepatobiliary retention of both dinorCDCA and norCDCA occurred, consistent with efficient ductular absorption (calculated to be 94%) and cholehepatic cycling of the unmetabolized bile acids. It is concluded that dinorCDCA, as norCDCA, is inefficiently amidated, is metabolized as a xenobiotic, and induces hypercholeresis. DinorCDCA is the first dihydroxy bile acid to be identified that is secreted largely in unconjugated form in bile.

IT 195205-20-0
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(effect of side chain length on biotransformation and hepatic transport and choleretic properties of chenodeoxycholyl homologs in rodent in relation to lipophilicity)

RN 195205-20-0 HCAPLUS

CN Pregnane-20-carboxylic acid, 7-hydroxy-3-oxo-, (5β,7α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1991:602975 HCAPLUS Full-text
DOCUMENT NUMBER: 115:202975
ORIGINAL REFERENCE NO.: 115:34541a,34544a
TITLE: Bioconversion of triterpenes by mycobacteria. Structure and conformation of the products of degradation of 7,11-dioxodihydrolanosterol by Mycobacterium phlei
AUTHOR(S): Jabbouri, Said; Chosson, Patricia; Tisnes, Pierre; Rao, Renee; Servin, Philippe; Prome, Jean Claude
CORPORATE SOURCE: Cent. Rech. Biochim. Genet. Cell., CNRS, Toulouse, 31062, Fr.

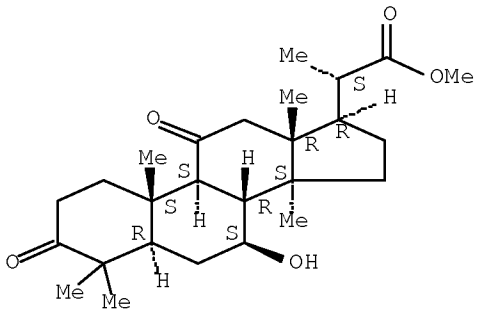
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1991), (8), 1935-40
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 15 Nov 1991

AB Although mycobacteria are unable to degrade lanosterol and dihydrolanosterol, principal components of wool fat, the transformation of some of their autoxidn. products by M. phlei was observed By analogy with the mechanism of cholesterol degradation, this difference was assumed to be due to the requirement for the presence of an enone group before the side-chain can be degraded. This paper reports the spectroscopic determination of the structure of the major metabolites of 7,11-dioxodihydrolanosterol. The side-chain is degraded from 8 carbon atoms to 3, the terminal carbon atom being oxidized to a primary alc. or a Me ester. The tetracyclic skeleton can undergo regioselective oxidation-reduction modifications at the 3- and 7-position. Their conformational anal., carried out by 2D-NMR methods, indicates a chair form for ring A of 3β-hydroxy derivs., while it is highly deformed for 3-keto compds. as predicted formerly by D. A. Dougherty, et al. (1979) for this lanostane series.

IT 136842-50-7 136842-51-8 136842-53-0
136842-54-1
RL: BIOL (Biological study)
(formation and conformation and structure of, of Mycobacterium phlei, as dioxodihydrolanosterol degradation product)

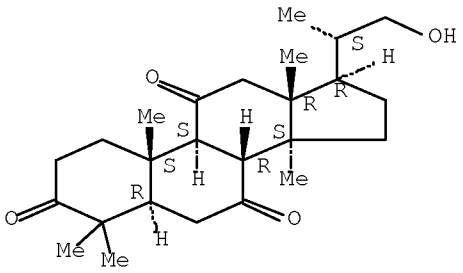
RN 136842-50-7 HCAPLUS
CN Pregnane-20-carboxylic acid, 7-hydroxy-4,4,14-trimethyl-3,11-dioxo-, methyl ester, (5α,7β,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



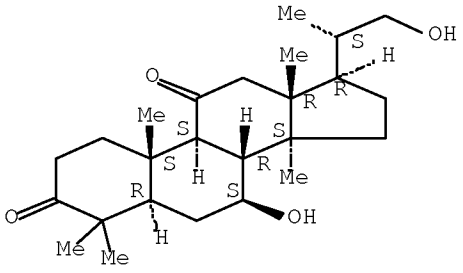
RN 136842-51-8 HCAPLUS
CN Pregnane-3,7,11-trione, 21-hydroxy-4,4,14,20-tetramethyl-, (5α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



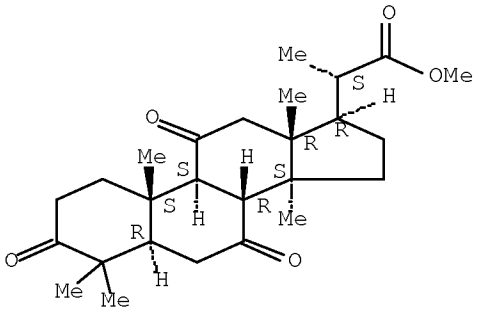
RN 136842-53-0 HCAPLUS
CN Pregnane-3,11-dione, 7,21-dihydroxy-4,4,14,20-tetramethyl-, (5α,7β,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 136842-54-1 HCAPLUS
CN Pregnane-20-carboxylic acid, 4,4,14-trimethyl-3,7,11-trioxo-, methyl ester, (5α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

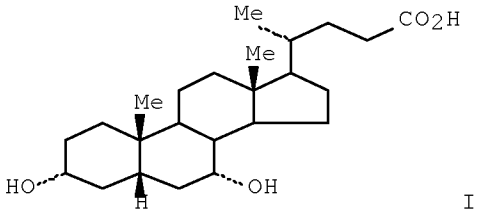


L8 ANSWER 15 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:407603 HCAPLUS Full-text
DOCUMENT NUMBER: 95:7603
ORIGINAL REFERENCE NO.: 95:1447a,1450a
TITLE: Chenodeoxycholic acid and intermediate products

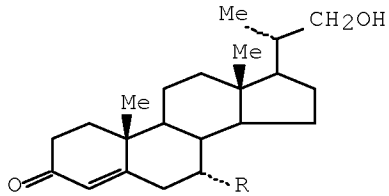
INVENTOR(S): Despreaux, Carl; Narwid, Thomas Albert; Palleroni, Norberto J.; Uskokovic, Milan R.
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.
SOURCE: Eur. Pat. Appl., 37 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
EP 18515	A2	19801112	EP 1980-101893		19800409	<--
EP 18515	A3	19810107				
EP 18515	B1	19821027				
R: AT, BE, CH, DE, FR, GB, IT, NL						
US 4230625	A	19801028	US 1979-29420		19790412	<--
US 4301246	A	19811117	US 1980-113019		19800118	<--
AT 1710	T	19821115	AT 1980-101893		19800409	<--
JP 56008399	A	19810128	JP 1980-47936		19800411	<--
PRIORITY APPLN. INFO.:			US 1979-29420	A	19790412	<--
			EP 1980-101893	A	19800409	<--

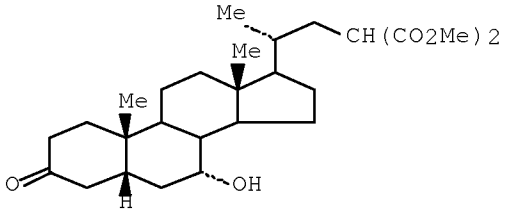
OTHER SOURCE(S): CASREACT 95:7603; MARPAT 95:7603
ED Entered STN: 12 May 1984
GI



I



II



III

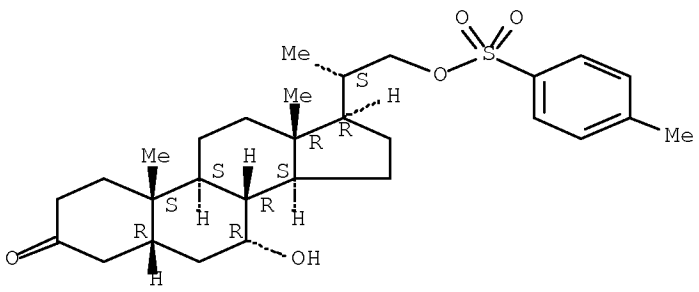
AB Chenodeoxycholic acid (I) was prepared from oxodinorcholenoic acid II (R = H). Thus, fermentation of II (R = H) with Botryodiplodia theobromae gave II (R = OH), which underwent consecutive hydrogenation, tosylation, and substitution reaction with CH2(CO2Me)2 to give norcholanedicarboxylate III. NaBH4 reduction of III and subsequent saponification-decarboxylation gave I.

IT 77530-53-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and substitution reaction with di-Me malonate)

RN 77530-53-1 HCAPLUS
CN Pregnan-3-one, 7-hydroxy-20-methyl-21-[[(4-methylphenyl)sulfonyl]oxy]-,

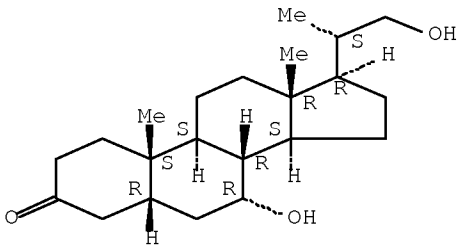
(5β,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 77530-52-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and tosylation of)
RN 77530-52-0 HCAPLUS
CN Pregnan-3-one, 7,21-dihydroxy-20-methyl-, (5β,7α,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 16 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1964:61153 HCAPLUS Full-text
DOCUMENT NUMBER: 60:61153
ORIGINAL REFERENCE NO.: 60:10750g-h
TITLE: Helvolic acid
AUTHOR(S): Okuda, Shigenobu; Iwasaki, Shigeo; Tsuda, Kyosuke; Sano, Yoshimoto; Hata, Toju; Udagawa, Shunichi; Nakayama, Yuya; Yamaguchi, Hiroshi
CORPORATE SOURCE: Univ. Tokyo
SOURCE: Chemical & Pharmaceutical Bulletin (1964), 12(1), 121-4
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.

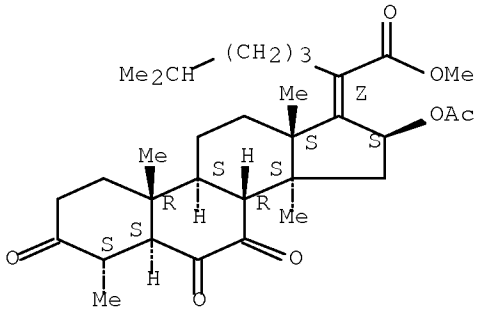
AB I was proposed as a partial structure for helvolic acid on the basis of chemical and spectral evidence. It was suggested that the remaining Me group was probably at C-14.

IT 107277-22-5, 29-Nordammar-17(20)-en-21-oic acid, 16β-hydroxy-3,6,7-trioxo-(?), methyl ester, acetate (preparation of)

RN 107277-22-5 HCAPLUS

CN 29-Nordammar-17(20)-en-21-oic acid, 16β-hydroxy-3,6,7-trioxo-, methyl ester, acetate (7CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L8 ANSWER 17 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:9147 HCAPLUS Full-text
DOCUMENT NUMBER: 55:9147
ORIGINAL REFERENCE NO.: 55:1845a-c
TITLE: Storage iron in the animal body. I. Alterations in storage iron following experimental bleeding, liver damage, and iron administration
AUTHOR(S): Yoshioka, Yuzo
CORPORATE SOURCE: Univ. Hiroshima Med. School
SOURCE: Hiroshima Igaku (1959), 10, 2565-74
CODEN: HIRGAY; ISSN: 0367-5904
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001

AB The changes in storage Fe in various organs of rabbits were studied under different conditions. In normal rabbits the ferritin (I) and hemosiderin (II) concns. were in the following order: spleen, liver, bone marrow, and kidney. The II content was higher than that of I in the liver, kidney, and bone marrow, while the reverse relation was observed in the spleen. Hemorrhagic anemia resulted in a marked decrease in storage Fe to a greater extent in spleen than in the liver, kidney, and bone marrow. In this case the predominant reduction was in I in the liver, spleen, and kidney, while II was more markedly reduced in the bone marrow. During the recovery phase after hemorrhage, a marked increase in liver II and a progressive decrease in I of all organs were observed. Recovery from the anemic state was much disturbed by the induction of liver damage, where a marked reduction of I and II occurred in the liver and spleen, and a slight decrease of I and a slight increase of II were seen in the kidney and bone marrow. Acceleration of recovery by Fe administration was accompanied by a marked increase in I and II in all organs. The increase was greatest in the liver.

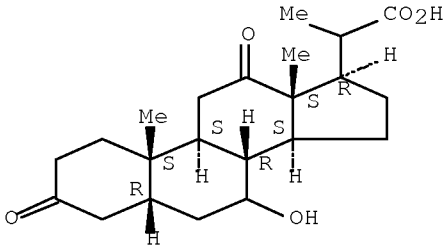
IT 111663-25-3

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 111663-25-3 HCAPLUS

CN 5β-Pregnane-20-carboxylic acid, 7-hydroxy-3,12-dioxo- (6CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 18 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1961:9146 HCAPLUS Full-text

DOCUMENT NUMBER: 55:9146

ORIGINAL REFERENCE NO.: 55:1844i,1845a

TITLE: The metabolism of bile acids. The metabolism of cholic acid and dehydrocholic acid by microorganisms

AUTHOR(S): Hoshita, Takahiko; Shimizu, Yoshimasa; Matsumura, Shinzo

CORPORATE SOURCE: Univ. Hiroshima Med. School

SOURCE: Hiroshima Igaku (1959), 10, 475-9

CODEN: HIRGAY; ISSN: 0367-5904

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

AB Cholate, when incubated with minced cat intestine, was metabolized to deoxycholate, while dehydrocholate was metabolized to 3,12-dioxo-7-hydroxybisnorcholanate.

IT 111663-25-3P, 5β-Pregnane-20-carboxylic acid, 7-hydroxy-3,12-dioxo-

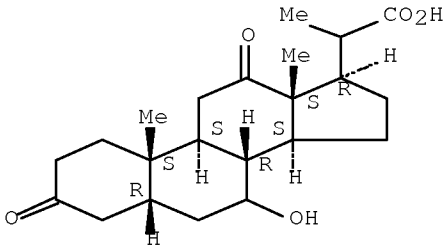
RL: PREP (Preparation)

(formation in dehydrocholic acid metabolism by intestinal bacteria)

RN 111663-25-3 HCAPLUS

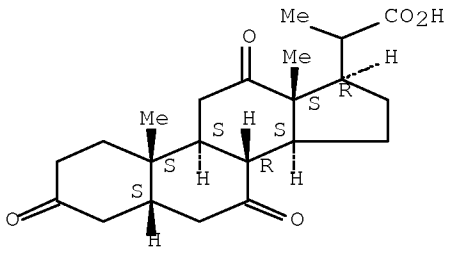
CN 5β-Pregnane-20-carboxylic acid, 7-hydroxy-3,12-dioxo- (6CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 19 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:8771 HCAPLUS Full-text
DOCUMENT NUMBER: 55:8771
ORIGINAL REFERENCE NO.: 55:1785c-d
TITLE: Metabolism of cholic acid, 3α,12α-dihydroxy-7-oxocholanic acid, and dehydrocholic acid by microorganisms
AUTHOR(S): Shimizu, Yoshimasa
CORPORATE SOURCE: Univ. Hiroshima Med. School
SOURCE: Hiroshima Igaku (1958), 9, 2243-50
CODEN: HIRGAY; ISSN: 0367-5904
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB The incubation of cholic acid with fresh dog intestinal homogenates gave rise to 3α,12α-dihydroxy-7-oxocholanic acid which was further metabolized to deoxycholic acid by one pathway and to dehydrobisnorcholic acid through dehydrocholic acid by another.
IT 102958-05-4P, 5β-Pregnane-20-carboxylic acid, 3,7,12-trioxo-
RL: PREP (Preparation)
(formation in cholic acid metabolism by intestinal microorganisms)
RN 102958-05-4 HCAPLUS
CN 5β-Pregnane-20-carboxylic acid, 3,7,12-trioxo- (6CI) (CA INDEX NAME)

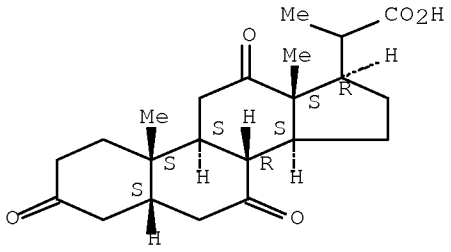
Absolute stereochemistry.



L8 ANSWER 20 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:8769 HCAPLUS Full-text
DOCUMENT NUMBER: 55:8769
ORIGINAL REFERENCE NO.: 55:1785a
TITLE: Metabolism of bile acids [by Aspergillus clavatus]
AUTHOR(S): Kameo, Hitoshi
CORPORATE SOURCE: Univ. Hiroshima Med. School
SOURCE: Hiroskima Igaku (1958), 9, 1541-3
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB Dehydrocholate was metabolized to β-reductodehydrocholate and dehydrobisnorcholate by A. clavatus in a modified Czapek medium.
IT 102958-05-4P, 5β-Pregnane-20-carboxylic acid, 3,7,12-trioxo-
RL: PREP (Preparation)
(formation from dehydrocholic acid by Aspergillus clavatus)
RN 102958-05-4 HCAPLUS

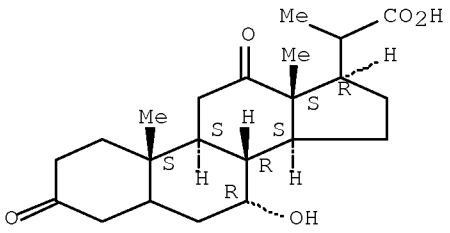
CN 5β-Pregnane-20-carboxylic acid, 3,7,12-trioxo- (6CI) (CA INDEX NAME)

Absolute stereochemistry.



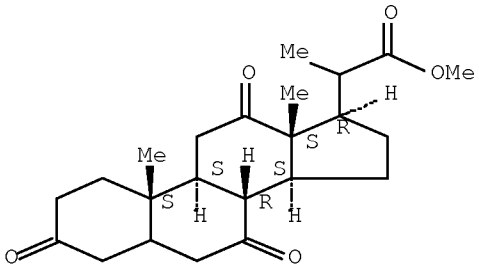
L8 ANSWER 21 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1956:1645 HCAPLUS Full-text
DOCUMENT NUMBER: 50:1645
ORIGINAL REFERENCE NO.: 50:388e-g
TITLE: Microbiological degradation of bile acid. III. Partial synthesis of methyl 7α-acetoxy-3,12-dioxobisnorcholanate from cholic acid
AUTHOR(S): Hayakawa, Shohei
CORPORATE SOURCE: Okayama Univ. Med. School
SOURCE: Proceedings of the Japan Academy (1954), 30, 139-42
CODEN: PJACAW; ISSN: 0021-4280
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 22 Apr 2001
AB Me 3α,7α-diacetoxy-12α-hydroxybischolanate (III), prepared from Me bisnorcholate by treatment with pyridine-Ac2O in benzene, m. 180-2° (sintering at 110°). III was converted to Me 7α-acetoxy-3α,12α-dihydroxybisnorcholanate (IV), m. 142°, by treatment with HCl in MeOH at 25-30°, followed by dilution with H2O, and recrystn. of the solids from benzene-petr. ether. IV with CrO3 in AcOH yielded Me 7α-acetoxy-3,12-dioxobisnorcholanate, m. 214-16°, giving a pos. Jaffe test, also prepared from the hydrogenated Me ester of I and Ac2O. 7α-Hydroxy-3,12-dioxobisnorcholanic acid, prepared from I by hydrogenation over Pd in EtOH, m. 249-52° and gave a positive Jaffe test; Me ester, prepared with CH2N2 in Et2O, m. 162-4° (sintering at 157°) (from EtOAc-petr. ether, then C6H6-petr. ether).
IT 911672-84-9, 20-Pregnanecarboxylic acid, 7α-hydroxy-3,12-dioxo-
(and esters)
RN 911672-84-9 HCAPLUS
CN 20-Pregnanecarboxylic acid, 7α-hydroxy-3,12-dioxo- (5CI) (CA INDEX NAME)

Absolute stereochemistry.



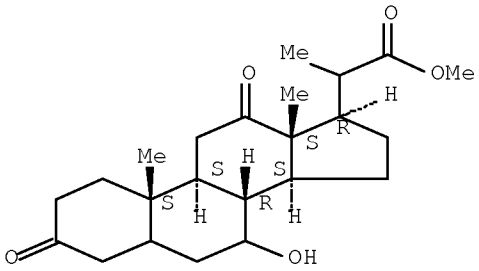
L8 ANSWER 22 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1956:1644 HCAPLUS Full-text
DOCUMENT NUMBER: 50:1644
ORIGINAL REFERENCE NO.: 50:388b-e
TITLE: Microbiological degradation of bile acid. II. Formation of 7-hydroxy-3,12-dioxobisnor-4,9(11)-choladienic acid from cholic acid by Actinomyces
AUTHOR(S): Hayakawa, Shohei
CORPORATE SOURCE: Okayama Univ. Med. School
SOURCE: Proceedings of the Japan Academy (1954), 30, 133-8
CODEN: PJACAW; ISSN: 0021-4280
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 22 Apr 2001
AB Cholic acid-containing media (see above) (20 l.) fermented by Actinomyces number 1164 was concentrated (after filtration to remove the microbial cells), the concentrate acidified with HCl, and chilled. After 20 hrs. at 0°, crystals were observed. These were recrystd. from MeOH (yield of 4 g. from 60 g. of cholic acid added to medium), and the dioxime, prepared from the Me ester of this acid (see previous paper), analyzed 5.97% N (oxime of 7-hydroxy-3,12-dioxobisnor-4,9(11)-choladienate analyzed 5.95% N). Hydrogenation of the Me ester gave needles (m. 166-9°) which gave a pos. Jaffe test and neg. Shimizu-Mizuhara test, and was tentatively identified as Me 7-hydroxy-3,12-dioxobisnorcholanate (II). The dioxime of II was prepared and m: 232-4°, N content, 6.53%. Me dehydrobisnorcholate, prepared from II by treatment with CrO3, m. 197-9°, identical with that of a synthetic sample; trioxime, m. 267-9°, N content, 9.57%, values similar to those obtained with synthetic materials. The ultraviolet spectra of the parent compound showed an absorption maximum at 240.3 mμ (ε = 11.15 + 104), and of the Me ester, 242.1 mμ (ε = 11.98 + 104). The data collected support the view that I is 7-hydroxy-3,12-dioxobisnor-4,9(11)-choladienic acid.
IT 881385-35-9P, 20-Pregnanecarboxylic acid, 3,7,12-trioxo-, methyl ester 911495-03-9P, 20-Pregnanecarboxylic acid, 7-hydroxy-3,12-dioxo-, methyl ester
RL: PREP (Preparation)
(preparation of)
RN 881385-35-9 HCAPLUS
CN 20-Pregnanecarboxylic acid, 3,7,12-trioxo-, methyl ester (5CI) (CA INDEX NAME)

Relative stereochemistry.



RN 911495-03-9 HCAPLUS
CN 20-Pregnanecarboxylic acid, 7-hydroxy-3,12-dioxo-, methyl ester (5CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 23 OF 23 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1956:1643 HCAPLUS Full-text
DOCUMENT NUMBER: 50:1643
ORIGINAL REFERENCE NO.: 50:387h-i,388a-c
TITLE: Microbiological degradation of bile acid. I. On β-oxidation and unsaturation of cholic acid by Actinomyces
AUTHOR(S): Hayakawa, Shohei
CORPORATE SOURCE: Okayama Univ. Med. School
SOURCE: Proceedings of the Japan Academy (1954), 30, 128-32
CODEN: PJACAW; ISSN: 0021-4280
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 22 Apr 2001
AB When Actinomyces number 1164 (Okayama Tobacco Laboratory, Japan Monopoly Bureau) was grown for 14 days (incubation temperature 30°) on a medium containing 6 g. cholic acid, 2 g. (NH4)2SO4, 2 g. K2HPO4, 1 g. MgSO4.7H2O, 0.02 g. FeCl3.6H2O, and 2 l. H2O (pH adjusted to 7.2 with NaOH) in culture without agitation (100 ml. medium/500 ml. conical flask) the pH dropped to 5.8, a neg. Pettenkofer test was obtained, and no precipitate was observed when the pH was lowered with HCl. The cell-free liquid was concentrated (at pH 7.2) in vacuo to about 0.1 volume, and 2 substances crystallized An acid (I), m. 280-2° (decomposition), gave neg. results to the Hammarsten-Yamasaki, the Mylius, and Shimizu-Mizuhara tests. A yellow Liebermann test was obtained, while pos. Jaffe and Zimmermann tests were obtained only after 5

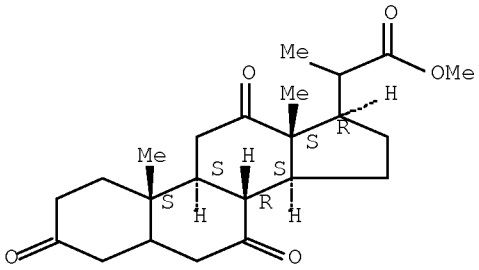
min. I was slightly soluble in H2O, MeOH, EtOH, and acetone, and insol. in Et2O, petr. ether, and benzene. Mol. weight from titration was 377.25; analysis for C22H28O5: C, 70.9; H, 7.58; found, C, 70.1; H, 8.01. The Me ester, prepared by treatment with CH2N2 in Et2O, m. 237° (sintering) (from MeOH). I was hydrogenated over Pt oxide, but oils were obtained. Oxidation of the Me ester with CrO3 in AcOH gave an ester identified as Me bisnorcholate by comparison with a sample prepared from cholic acid by the procedure of Morsman, et al. (C.A. 31, 3062.4). A second acid from the fermentation C20-24H28-34O5-6, m. 248° (decomposition), and had the same qual. tests and solubilities as the other acid.

IT 881385-35-9P, 20-Pregnanecarboxylic acid, 3,7,12-trioxo-, methyl ester
RL: PREP (Preparation)
(preparation of)

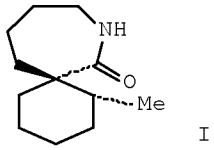
RN 881385-35-9 HCAPLUS

CN 20-Pregnanecarboxylic acid, 3,7,12-trioxo-, methyl ester (5CI) (CA INDEX NAME)

Relative stereochemistry.



L26 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:61598 HCAPLUS Full-text
DOCUMENT NUMBER: 150:214146
TITLE: Synthesis of Enantiopure Bicyclic α,α-Disubstituted Spirolactams via Asymmetric Birch Reductive Alkylation
AUTHOR(S): Gueret, Stephanie M.; O'Connor, Patrick D.; Brimble, Margaret A.
CORPORATE SOURCE: Department of Chemistry, University of Auckland, Auckland, N. Z.
SOURCE: Organic Letters (2009), 11(4), 963-966
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 16 Jan 2009
GI



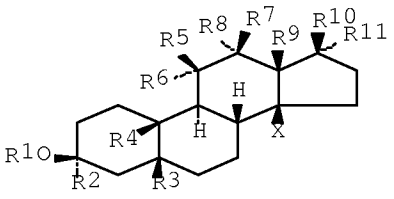
I

AB The synthesis of enantiopure bicyclic α,α-disubstituted spirolactams is described using a diastereoselective Birch reductive alkylation as the key step. Hydrogenation of the resultant alkylated cyclohexadienes followed by intramol. cyclization provides access to enantiopure 8-azaspiro[5.6]dodecan-7-ones, e.g. I.
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

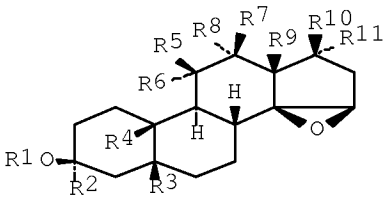
L26 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:100362 HCAPLUS Full-text
DOCUMENT NUMBER: 143:44004
TITLE: Total synthesis of 14 beta-fluorosteroids via the transannular Diels-Alder reaction
INVENTOR(S): Beaubien, Sylvie; Deslongchamps, Pierre
PATENT ASSIGNEE(S): Neokimia Inc., Can.
SOURCE: Can. Pat. Appl., 321 pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2418458	A1	20040806	CA 2003-2418458	20030206
PRIORITY APPLN. INFO.:			CA 2003-2418458	20030206

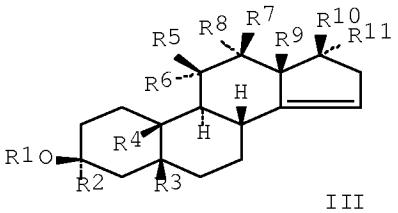
OTHER SOURCE(S): MARPAT 143:44004
ED Entered STN: 04 Feb 2005
GI



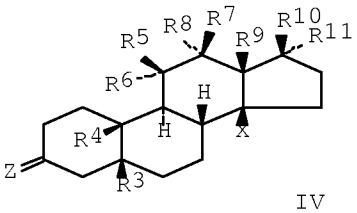
I



II



III



IV

AB A series of novel digitalis steroid analogs, including derivs. containing a 14β-fluoro substituent, I [R1 = H, Me, C2-6-alkyl (optionally substituted with NRbRc or NHC(:NRd)NRbRc], (un)substituted (CH2)nPh, C(:O)Ra, mono-, di-, trisaccharyl, aminoacyl, di-, tripeptidyl ; R2 = H, Me, OR1; R3 = H, Me, ORd, OC(:O)Rd; R4 = H, Me, OC(:O)Rd, CHO, (CH2)mORd, (CH2)nNRbRc; R5, R6, R7, R8 = H, ORd, OC(:O)Rd; R9 = H, Me; R10 = H, (CH:CR9)p(CH2)m(CHR9)nA, (CH:CR9)p(CHR12)(CHR9)nA, (CHR9)m(CH:CR9)pB, furyl derivative, furanone derivative, pyranone derivative, pyrazin-4-yl; R11 = H, ORa, OC(:O)Ra; R12 = ORg, NRhRi; NHC(:Y)NRhRi; Rg = Ra; Rh, Ri = Ra with the proviso that, when Rh = H, Ri = NHC(:NH)NH2; Y = O, S, NRa; Ra = H, Me, C2-6-alkyl (optionally substituted with NRbRc or NHC(:NRd)NRbRc), (un)substituted (CH2)nPh; Rb, Rc = H, Me, C2-6-alkyl, (un)substituted (CH2)nPh; NRbRc = 5- or 6-membered monoheterocyclic ring, optionally containing N or O; Rd = H, Me, C2-6-alkyl, (un)substituted (CH2)nPh; X = Fl, Cl, Br, I; A = NO2, CO2Ra, CHO, R12, CR9:NR12; B = NO2, CO2Ra, CHO, CR9:NR12; m = 0-6; n = 1-6; p = 0-3), II, III and IV [Z = O, S, NR12], their tautomers, R/S-enantiomers (excluding the steroid nucleus), or E/Z double bonds isomers, have been synthesized. I-IV have been shown to display binding affinity for the ouabain receptor as well as activity in the inhibitions of Na+,K+-ATPase. These compds. have implications in therapy for a number of medical indications, most notably congestive heart failure, hypertension and cancer. In addition, these mols. can function as natriuretic/diuretic agents and neuromodulators. Multiple methods for the synthesis of these compds. are also presented.

L26 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:583184 HCAPLUS Full-text
DOCUMENT NUMBER: 131:199937
TITLE: Preparation of deoxymannojirimycin from (4R)-3-benzyl-4-(methoxycarbonyl)-2-oxazolidinone
INVENTOR(S): Katsumura, Shigeo; Asano, Hiroshi; Murakami, Masanobu; Iwama, Seiji
PATENT ASSIGNEE(S): Daiso Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11246524	A	19990914	JP 1998-43381	19980225
JP 3317233	B2	20020826		

PRIORITY APPLN. INFO.: JP 1998-43381 19980225
OTHER SOURCE(S): CASREACT 131:199937; MARPAT 131:199937
ED Entered STN: 16 Sep 1999
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Deoxymannojirimycin, a known anticancer and antiviral agent, is prepared from (4R)-3-benzyl-4-(methoxycarbonyl)-2-oxazolidinone (I; R = OMe) without using expensive and difficult-to-handle reagents in a highly stereoselective method. The process involved treatment of O-(tert -butyldimethylsilyl)propargyl alc. with BuLi in THF/hexamethylphosphoramide at -78° for 1 h and coupling with (4R)-3-benzyl-4-(methoxycarbonyl)-2-oxazolidinone (I; R = OMe) at -100° for 15 min to give propynyl ketone (I; R = tert-BuMe2SiOCH2C.tplbond.C) (65.5%), reduction of the latter ketone with diisobutylaluminum-2,6-di-tert-butyl-4-methylphenoxide in toluene at 0° for 10 min to 4-(1,4-dihydroxy-2-butynyl)oxazolidinone (II) (92.2%), hydrogenation of the latter compound over Lindlar catalyst to N-benzyl-4-(cis-1,4-dihydroxy-2-butenyl)oxazolidinone (III; R1 = CH2Ph, R2 = H, R3 = tert-BuMe2Si)(100%), Birch reduction of the N-benzyloxazolidinone with Na in NH3(l) at -78° to give 4-(cis-1,4-hydroxy-2-butenyl)oxazolidinone (III; R1 = R2 = H, R3 = tert-BuMe2Si)(79.9%), silylation of the latter alc. with tert- butyldimethylsilyl chloride in the presence of imidazole in DMF (96.4%) and selective desilylation with a mixture of 33% aqueous HF and MeCN at -20° for 30 min to give III (R1 = R3 = H, R2 = tert-BuMe2Si) (97.6%). Mesylation of the latter compound with methanesulfonyl chloride 4-dimethylaminopyridine and Et3N in DMF followed by treatment of the crude mesylate (III; R1 = H, R2 = tert-BuMe2Si, R3 = SO2Me) with NaH in DMF at 0° for 1 h gave a bicyclic oxazolidinone derivative (IV) (79.9%) which underwent OsO4-catalyzed dihydroxylation with N-methylmorpholine-N-oxide in a mixture of tert-Bu alc. and H2O at 0° to a diol (V; R4 = H) (85.6%). Acetonation of the latter diol with 2,2-dimethoxypropane in acetone in the presence of pyridinium p-toluenesulfonate at room temperature for 20 h gave an acetonide (V; R4R4 = Me2C) (92.1%) which was refluxed with a mixture of 6 N aqueous NaOH and dioxane for 2 days to 70.7% give deoxymannojirimycin acetonide (VI). Deacetonation was effected by refluxing the latter acetonide in MeOH in the presence of concentrated H2SO4 followed by purification on an ion exchange column (I-X4, OH- form) to give 76.5% deoxymannojirimycin.

L26 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:512071 HCAPLUS Full-text
DOCUMENT NUMBER: 140:253359
TITLE: An efficient synthesis of pironetins employing a useful chiral building block, (1S,5S,6R)-5-hydroxybicyclo[4.1.0]heptan-2-one
AUTHOR(S): Watanabe, Hidenori; Watanabe, Hiroyuki; Bando,

Masahiko; Kido, Masaru; Kitahara, Takeshi
CORPORATE SOURCE: Department of Applied Biological Chemistry, Graduate School of Agricultural and Life Sciences, The University of Tokyo, Tokyo, 113-8657, Japan
SOURCE: Tetrahedron (1999), 55(32), 9755-9776
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:253359
ED Entered STN: 18 Aug 1999
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A convergent total synthesis of pironetin (I; R = Me) and related compound I (R = H) using a chiral building block, (1S,5S,6R)-5-hydroxybicyclo[4.1.0]heptan-2-one (II) is described. Both the dithiane III and the epoxide IV with proper substituents were employed as coupling partners to construct the whole carbon skeleton V, which was converted to (-)-pironetin (I; R = Me) and (-)-I (R = H) in few steps. The usefulness of II for polyketide synthesis was demonstrated.
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:299594 HCAPLUS Full-text
DOCUMENT NUMBER: 125:58151
ORIGINAL REFERENCE NO.: 125:11177a,11180a
TITLE: Synthesis of 3-[1-(tert-butyldimethylsilyloxy)ethyl]-4-carboxymethyl-2-azetidinone derivatives
AUTHOR(S): Seo, Min Hyo; Lee, Youn Young; Goo, Yang Mo
CORPORATE SOURCE: Department Chemistry, Seoul National University, Seoul, 151-742, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1996), 17(4), 314-321
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:58151
ED Entered STN: 21 May 1996
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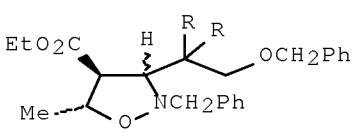

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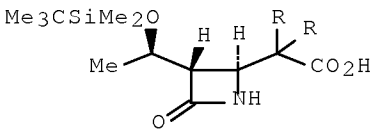

II

AB Isoxazolidine derivs. I (R = H, Me) were synthesized from N-benzyl-C-(2-benzyloxyethyl)nitrones by 1,3-dipolar cycloaddn. with (E)-Et crotonate. The

isoxazolidine derivs. were converted to β-amino acid esters by reduction with zinc in acetic acid. The β-amino acid esters were reacted with methylmagnesium bromide to give the 2-azetidinones. The benzyl group of 2-azetidinones were removed by Birch reduction The products were oxidized with PDC to give 3-[1-(t-butyldimethylsilyloxy)ethyl]-4-carboxymethyl-2-azetidinone derivs II (R = H, Me).

L26 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:603806 HCAPLUS Full-text
DOCUMENT NUMBER: 119:203806
ORIGINAL REFERENCE NO.: 119:36373a,36376a
TITLE: A novel constrained reduced-amide inhibitor of HIV-1 protease derived from the sequential incorporation of γ-turn mimetics into a model substrate
AUTHOR(S): Newlander, Kenneth A.; Callahan, James F.; Moore, Michael L.; Tomaszek, Thaddeus A., Jr.; Huffman, William F.
CORPORATE SOURCE: Dep. Med. Chem., SmithKline Beecham Pharm., King of Prussia, PA, 19406, USA
SOURCE: Journal of Medicinal Chemistry (1993), 36(16), 2321-31
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:203806
ED Entered STN: 13 Nov 1993
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB C7 mimetics, designed to lock three amino acid residues of a peptide chain into a γ-turn conformation, were introduced sequentially between the P3 to P2' positions of a model HIV-1 protease substrate I resulting in compds. I, II and III as probes for conformational requirements in binding to HIV-1 protease. The above I-III were obtained as 2 diastereoisomers. A diastereoisomer of II with the C7 mimetic replacing Asn-Tyr-Pro, corresponding to the P2 through P1' positions of substrate, was found to be an inhibitor with a Ki of 147 μM. Reduction of the amide bond in the C7 mimetic of the above diastereoisomer of II resulted in a novel constrained reduced-amide mimetic IV with a Ki of 430 nM. This corresponds to over a 300-fold improvement in inhibitory activity over the original C7 mimetic. The inhibitory activity of mimetic IV was in addition found to be 44-fold better than a similar linear reduced-amide containing inhibitor H-Ser-Ala-Ala-Pheψ[CH2N]Pro-Val-Val-NH2. The synthesis of these mimetics are described.

L26 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:119219 HCAPLUS Full-text
DOCUMENT NUMBER: 112:119219
ORIGINAL REFERENCE NO.: 112:20211a,20214a
TITLE: A new bis-annelation method. Application to steroid synthesis
AUTHOR(S): Poirier, Jean Marie; Hennequin, Laurent
CORPORATE SOURCE: Lab. Chim. Org., Fac. Sci. Tech. Rouen, Mont Saint Aignan, 76134, Fr.
SOURCE: Tetrahedron (1989), 45(13), 4191-202

CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:119219
ED Entered STN: 31 Mar 1990
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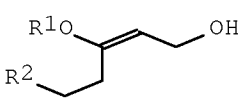

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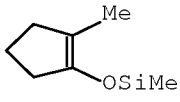

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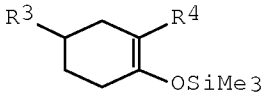

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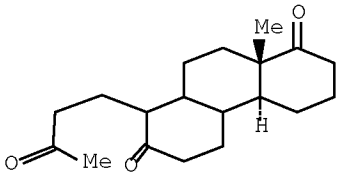

IV

AB New bis-annelation reagents I [R1 = tert- butyldimethylsilyl, R2 = (2-methyl-2-dioxolanyl)methyl, MeC(:CH2)CH2; R1 = Me, R2 = CH2:CHCH2] and R2CH2CH2COCH:CH2 (R2 = same) are described. With monocyclic enolates equivalent II and III (R2 = H, R3 = Me; R2 = CMe3, R3 = H), these reagents led to the formation of tricyclic compds. in few steps. The utility of the method is tested for the steroid rings synthesis. Thus, triketone IV was prepared

L26 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1987:195930 HCAPLUS Full-text
DOCUMENT NUMBER: 106:195930
ORIGINAL REFERENCE NO.: 106:31748h,31749a
TITLE: Improved methods for the reductive alkylation of methoxybenzoic acids and esters. Applications to the synthesis of bicyclic ketones
AUTHOR(S): Hamilton, Robert J.; Mander, Lewis N.; Sethi, S. Paul
CORPORATE SOURCE: Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SOURCE: Tetrahedron (1986), 42(11), 2881-92
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:195930
ED Entered STN: 13 Jun 1987
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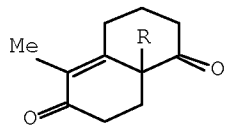

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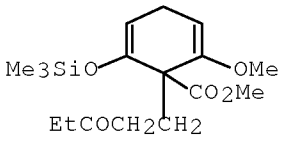

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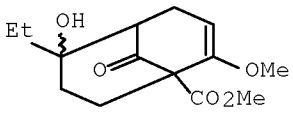

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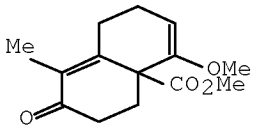

IV

AB A series of methoxybenzoic acids and esters was reduced by metal-NH3 solns. and the resulting 1,4-dihydro products were either alkylated in situ or isolated and alkylated subsequently. Three different types of alkyl iodides were employed to introduce the elements of a butanone or pentanone side-chain as a prelude to adding a fused six-membered ring, thereby completing the preparation of several analogs of the Wieland-Miescher ketone I (R = H), in which the angular substituent was oxygenated. Thus, 2,6-MeO(Me3SiO)C6H3CO2Me was treated sequentially with K-Me3COH in NH3, LiBr, and then ICH2CH2CH(OSiMe3)CH2Me, followed by Me2SO and DCC to give 60% the cyclohexadienecarboxylate II. Treating II with Bu4NF in THF gave up to 90% diastereomeric bicyclononenecarboxylates III, which rearranged on treatment with K2CO3 in MeOH to give 75% bicyclodecadienecarboxylate IV. Demethylation of IV with Hg(NO2)2 in MeCN-H2O gave 91% I (R = CO2Me).

SEARCH HISTORY

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     FILE 'CASREACT' ENTERED AT 14:16:38 ON 10 MAR 2009
L1              STRUCTURE UPLOADED
L2            0 SEA SSS SAM L1 (     0 REACTIONS)
L3            1 SEA SSS FUL L1 (     3 REACTIONS)

     FILE 'REGISTRY' ENTERED AT 14:23:55 ON 10 MAR 2009
L4              STRUCTURE UPLOADED
L5            0 SEA SSS SAM L4
L6           22 SEA SSS FUL L4

     FILE 'HCAPLUS' ENTERED AT 14:29:17 ON 10 MAR 2009
L7           23 SEA SPE=ON  ABB=ON  PLU=ON  L6
L8           23 SEA SPE=ON  ABB=ON  PLU=ON  L7 AND (PRY<=2005 OR AY<=2005 OR
                PY<=2005)
L9           25 SEA SPE=ON  ABB=ON  PLU=ON  KOYAKUMARU K?/AU
L10         227 SEA SPE=ON  ABB=ON  PLU=ON  SUGIOKA T?/AU
L11          10 SEA SPE=ON  ABB=ON  PLU=ON  OHZONO S?/AU
L12        1278 SEA SPE=ON  ABB=ON  PLU=ON  NAKAGAWA N?/AU
L13           7 SEA SPE=ON  ABB=ON  PLU=ON  (L9 OR L10 OR L11 OR L12) AND L8
L14           2 SEA SPE=ON  ABB=ON  PLU=ON  L9 AND L10 AND L11 AND L12
L15           3 SEA SPE=ON  ABB=ON  PLU=ON  L12 AND L9
L16           2 SEA SPE=ON  ABB=ON  PLU=ON  L12 AND L10
L17           2 SEA SPE=ON  ABB=ON  PLU=ON  L12 AND L11
L18           3 SEA SPE=ON  ABB=ON  PLU=ON  (L14 OR L15 OR L16 OR L17)
L19        1485 SEA SPE=ON  ABB=ON  PLU=ON  BIRCH REDUCTION/CT OR BIRCH
                REDUCTION/BI
L20           0 SEA SPE=ON  ABB=ON  PLU=ON  L8 AND L19
L21           0 SEA SPE=ON  ABB=ON  PLU=ON  L19 AND (L9 OR L10 OR L11 OR L12)
L22         575 SEA SPE=ON  ABB=ON  PLU=ON  METAL LITHIUM/BI
L23           0 SEA SPE=ON  ABB=ON  PLU=ON  L19 AND L22
L24           0 SEA SPE=ON  ABB=ON  PLU=ON  L22 AND (L9 OR L10 OR L11 OR L12)
L25        7329 SEA SPE=ON  ABB=ON  PLU=ON  TERT BUTYLDIMETHYLSILYL/BI OR
                T-BUTYLDIMETHYLSILYL/BI
L26           8 SEA SPE=ON  ABB=ON  PLU=ON  L19 AND L25
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